A universal scheme for robust self-testing in the prepare-and-measure scenario

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We consider the problem of certification of arbitrary ensembles of pure states and projective measurements solely form the experimental statistics in the prepare-and-measure scenario assuming the upper bound on the dimension of the Hilbert space. To this aim we propose a universal and intuitive scheme based on establishing perfect correlations between target states and suitably-chosen projective measurements. The method works in all finite dimensions and allows for robust certification of the overlaps between arbitrary preparation states and between the corresponding measurement operators. Finally, we prove that for qubits our technique can be used to robustly self-test arbitrary configurations of pure quantum states and projective measurements. These results pave the way towards practical application of the prepare-and-measure paradigm to certification of quantum devices.

Quantum devices are becoming more and more complex and the possibilities of their precise control and manipulation keep increasing. Recently reported demonstration of quantum computational advantage by Google \cite{arXiv:2003.01032v3} is only an intermediate milestone and quantum technologies have a potential real-life applications in fields such as quantum sensing, efficient computation and machine learning. \cite{arXiv:2003.01032v3}

With the increasing complexity of quantum systems, there is a growing need for certification and verification of their performance. This task is usually realized via the combination of quantum tomography and various benchmarking schemes (see \cite{arXiv:2003.01032v3} for a recent review). However, these methods, despite being powerful and universally applicable, depend on the assumptions about the inner workings of quantum systems, such as perfect measurements or uncorrelated and independent errors. In contrast to these approaches self-testing is a method which aims at proving the uniqueness of the implemented states or measurements based solely on the observed statistics and under minimal physical assumptions.

The paradigm of self testing was first introduced in the context of quantum cryptography \cite{arXiv:2003.01032v3}, with the aim to obtain trust in cryptographic devices (see \cite{arXiv:2003.01032v3} for a recent review). It was initially applied to correlations observed in the Bell scenario \cite{arXiv:2003.01032v3} (see e.g. \cite{arXiv:2003.01032v3} \cite{arXiv:2003.01032v3} \cite{arXiv:2003.01032v3} \cite{arXiv:2003.01032v3}). The most know result is certification of the singlet state in the case of maximal violation of the CHSH Bell inequality \cite{arXiv:2003.01032v3}. Recently, there is also a lot of interest in prepare-and-measure scenarios that are more experimentally appealing (see e.g. \cite{arXiv:2003.01032v3} \cite{arXiv:2003.01032v3}). Therein, unlike in the Bell scenario, one does not need to ensure space-like separation of the measurement events by two parties. In contrast, one party, Alice, communicates some of her states to Bob, who measures them. In order to get meaningful certification results further assumptions are needed.

In the most commonly studied semi-device-independent (SDI) scenario \cite{arXiv:2003.01032v3}, one assumes that the dimension of the quantum system used for transmitting information is bounded from above. There exist, however, alternative approaches based on other constraints like minimal overlap \cite{arXiv:2003.01032v3}, mean energy constraint \cite{arXiv:2003.01032v3} or entropy constraint \cite{arXiv:2003.01032v3}.

Recently, there was a lot of interest in self-testing and certification in SDI setting. First, self-testing results were proven for mutually unbiased bases (MUBs) in dimension 2, for both state ensembles and measurements \cite{arXiv:2003.01032v3}. This was further generalised to SDI certification of mutual unbiasedness of pairs of bases in an arbitrary dimension in \cite{arXiv:2003.01032v3}. Furthermore, methods for self-testing of extremal qubit POVMs were proposed in \cite{arXiv:2003.01032v3} \cite{arXiv:2003.01032v3} and further extended to symmetric-informationally complete (SIC) POVMs \cite{arXiv:2003.01032v3}. Importantly, the above results either rely on numerical approaches (for general state preparations and POVMs) or work only for special scenarios that exhibit many symmetries.

In this work we propose a simple analytical method allowing to certify overlaps between preparations of arbitrary pure states and arbitrary projective measurements in qudit systems. The scheme relies on establishing perfect correlations between preparation states and outcomes of suitably-chosen projective measurements. The method is universally applicable and robust to experimental noise. We prove that for qubits our SDI certification method can be used to obtain a robust self-testing result for arbitrary preparations of pure qubit states and corresponding projective measurements. While for higher dimensions we do not show self-testing, our scheme allows for SDI certification of many features..
relevant for quantum information processing such as: arbitrary overlaps between two measurement bases or SIC relations among measurement effects.

We believe that our findings greatly extend the applicability of the paradigm of self-testing in the SDI setting. They will likely have application for certification of near-term quantum computers \cite{7}, especially since our scheme is not sensitive to state-preparation and measurement errors, which is one of the major problems in certification of quantum devices \cite{27}. We also expect possible cryptographic applications as our setup is very similar to the one of textbook quantum key distribution schemes \cite{28, 29}. The perfect correlations can be utilized for generation of the secret key while the rest can be used to estimate the security. Thus our methods can be directly applied for certification of quantum devices implementing protocols such as BB84 \cite{28} which is normally achieved by introducing additional preparation states or measurement bases \cite{30}.

Notation.— Let $X$ be a linear operator acting on a finite-dimensional Hilbert space $\mathcal{H}$. Throughout the paper we use $\|X\|$, $\|X\|_F$ to denote operator norm and Frobenius norm of $X$. We will also use $[n]$ to denote the Euclidean norm of $n \in \mathbb{R}^3$, and $[n]$ to denote an $n$-element set $\{1, 2, \ldots, n\}$.

Description of the scenario.— We consider a prepare-and-measure scenario in which in each run of the experiment Alice prepares a quantum $d$-level system in one of the states from a finite set of preparations $\rho_a^x$ for which we use two indexes $x \in [n]$ and $a \in [d]$. Subsequently, Bob performs a measurement on this state with a finite choice of measurement settings $y \in [n]$ having the possible outcomes $b \in [d]$. We assume that measurement processes performed by Bob is described by quantum mechanics and furthermore that the parties do not communicate in any other way and do not have access to any entangled states or shared randomness \cite{31} (the role of this assumption is discussed in detail later in the text). This implies that the observed statistics $p(b|a, x, y)$ are given by the Born rule i.e. $p(b|a, x, y) = \text{tr}(\rho_a^x M_b^y)$, where $M^y = (M_b^1, M_b^2, \ldots, M_b^n)$ is a quantum measurement (POVM) performed by Bob upon the choice of the setting $y$. The idea of SDI certification is then to identify certain properties of states or measurements based solely on the observed statistics $p(b|a, x, y)$ assuming the upper bound on the dimension $d$ and the validity of Born’s rule. We say that certain states $\rho_a^x$ and measurements $M^y$ can be self-tested if the observed statistics specify these objects uniquely up to a unitary transformation and, perhaps, a global transposition.

Certification of overlaps.— We start with a presentation of our scheme for certifying pairwise overlaps between pure qudit preparation states and between the corresponding projective measurements. By “corresponding” we mean that in our scheme we set these states and measurements to be “equal” in a sense that $\rho_a^x = (\rho_a^x)^{1/2} = M_b^y$ for all $a \in [d]$ and $x \in [n]$. In what follows we will refer to these objects as target pure states and target measurements respectively. Their experimental counterparts we denote as $\tilde{\rho}_a^x$, and $\tilde{M}^y$ respectively. By “experimental” we mean any states and measurements defined over the same Hilbert space as the target ones and that reproduce the observed statistics i.e. $\tilde{p}(b|a, x, y) = \text{tr}(\tilde{\rho}_a^x \tilde{M}_b^y)$. Clearly, we do not assume that the experimental states and measurement have to be “equal”.

The idea of our certification scheme is very intuitive, yet powerful (see Fig. 1). Assume that Alice and Bob prepared their devices in a way that $\tilde{p}(b|a, x, y) = 1$, whenever $y = x$ and $b = a$. In other words, outcomes of Bob’s measurement are perfectly correlated with the preparations of Alice (whenever $x = y$). Since the quantum dimension is upper bounded by $d$, we can easily conclude that $\tilde{\rho}_a^x = M_b^x$, for all $a \in [d]$ and $x \in [n]$. Clearly, after these perfect correlations are established, the “cross-terms”, can be used to compute the overlaps between the preparation states and between measurement operators: $\tilde{p}(b|a, x, y) = \text{tr}(\tilde{\rho}_a^x \tilde{M}_b^y) = \text{tr}(\tilde{\rho}_b^y \tilde{M}_a^x) = \text{tr}(M_b^x M_a^y)$. Therefore, if the experimental statistics $\tilde{p}(b|a, x, y)$ match the target statistics $p(b|a, x, y)$, we can certify that overlaps between experimental states match those of the target states. The same holds for the corresponding measurement operators.

Our method can be also applied when experimental statistics do not match exactly the target ones.

**Theorem 1** (Robust SDI certification of overlaps). Consider pure target qudit preparation states $\rho_a^x$ and target projective measurements $M^y$, where $a \in [d]$ and $x, y \in [n]$. Assume that $\rho_a^x = M_b^y$ for all $a, x$ and furthermore that experimental states $\tilde{\rho}_a^x$ and measurements $\tilde{M}^y$ act on Hilbert space of dimension at most $d$ and generate statistics $\tilde{p}(b|a, x, y) = \text{tr}(\tilde{\rho}_a^x \tilde{M}_b^y)$ such that $|\tilde{p}(b|a, x, y) - \text{tr}(\tilde{\rho}_b^y \tilde{M}_a^x)| \leq \varepsilon$, for all $a, b, x, y$. Then, input states $\tilde{\rho}_a^x$ are almost pure and measurements $\tilde{M}^y$ are almost projective in the sense that

$$\sum_{a=1}^{d} \|\tilde{\rho}_a^x\| \geq d(1 - 2\varepsilon) \quad (1)$$

Moreover, for all $x \neq x', a \neq a', y \neq y'$, and $b \neq b'$, we have

$$\sum_{b=1}^{d} \|\tilde{M}_b^{y'} - \tilde{M}_b^{y}\| \geq d(1 - \varepsilon) \quad (2)$$
have
\[
|\text{tr}(\tilde{\gamma}_a^x \tilde{\gamma}_b^x) - \text{tr}(\tilde{\gamma}_a^y \tilde{\gamma}_b^y)| \leq \varepsilon + \sqrt{2\varepsilon + d^2\varepsilon^2},
\]
\[
|\text{tr}(M_b^y \tilde{M}_b^y) - \text{tr}(M_b^y \tilde{M}_b^y)| \leq \varepsilon + (1 + d\varepsilon)\sqrt{2\varepsilon + d^2\varepsilon^2}.
\]

The above result states that if the statistics observed in our certification scheme vary just a little bit from the target ones, the overlaps of the experimental states are also close to the overlaps between target states (and analogously for measurements). To our best knowledge analogous results have been previously known only for very special symmetric target states and measurements forming MUBs [22, 23]. We give the formal proof of Theorem 1 in Appendix A. There, we also present improved bounds for the special case of qubits. Moreover, in Appendix B we prove, by giving explicit examples, that the bounds in Eq. (3) are tight in the first orders in $\sqrt{\varepsilon}$ and $d$.

Self-testing of qubits.– Certification of overlaps allows to prove robust self-testing result for arbitrary pure qubit preparations and projective measurements appearing in our certification scheme.

**Theorem 2** (Ideal self-testing of qubit systems). Consider target pure qubit states $\gamma_a^x$ and projective measurements $M_b^y$, where $a = 1, 2$ and $x,y \in [n]$. Assume that $\tilde{\gamma}_a^x = M_a^x$ for all $a,x$ and furthermore that experimental qubit states and measurements $\tilde{\gamma}_a^x, \tilde{M}_b^y$, reproduce the target statistics, i.e. $\text{tr}(\tilde{\gamma}_a^x \tilde{M}_b^y) = \text{tr}(\gamma_a^x M_b^y)$ for all $a,b,x,y$. Then, there exist a qubit unitary matrix $U$ such that for all $a,b,x,y$
\[
U(\tilde{\gamma}_a^x)^{(T)} U^\dagger = \gamma_a^x,
\]
\[
U(\tilde{M}_b^y)^{(T)} U^\dagger = M_b^y,
\]
where $(\cdot)^{(T)}$ stands for the transposition with respect to a fixed basis in $\mathbb{C}^2$ that may have to be applied to all experimental states and measurements at the same time.

**Proof.** We start by recalling the Bloch representation [32] of a qubit density matrix $\rho = \frac{1}{2}(1 + n \cdot \sigma)$, where $\sigma$ is the vector of Pauli matrices, and $|n| \leq 1$. As discussed in the previous section, from the assumption of Theorem 2 it follows that for all $x,x',a,a'$ we have $\tilde{\gamma}_a^x = \tilde{M}_a^x$ and $\text{tr}(\tilde{\gamma}_a^x \tilde{\gamma}_b^y) = \text{tr}(\gamma_a^x M_b^y)$. Using the Bloch representation, we can conclude that also $\tilde{n}_a^x \cdot \tilde{n}_b^y = n_a^x \cdot n_b^y$, where $n_a^x$ and $n_b^y$ are Bloch vectors of $\gamma_a^x$ and $\gamma_b^y$ respectively.

Assume now that the vectors $n_1^x, n_2^x, n_3^x$ are linear independent. Let $O$ be a linear transformation defined by $On_1^x = \tilde{n}_1^x$, $x = 1, 2, 3$, and let $L$ be a matrix whose rows are the vectors $n_1^x$, $x = 1, 2, 3$. Then, we have $LO^T OL^T = LL^T$, and consequently, since $L$ is invertible by the construction, $O^T O = I_3$, i.e. $O$ is an orthogonal transformation in $\mathbb{R}^3$. It is well-known [32] that if $\det(O) = 1$, there exist a unitary matrix $U$ satisfying Eq. (4) (without transposition) for the states corresponding to $x = 1, 2, 3$ and $a = 1$. By our assumption all remaining states $\gamma_a^x$ can be decomposed in the basis $\{1, \gamma_1^1, \gamma_1^2, \gamma_1^3\}$, with the coefficients depending solely on the overlaps $\text{tr}(\tilde{\gamma}_a^x \tilde{\gamma}_b^y)$. Hence, the same unitary $U$ that maps $\tilde{\gamma}_a^x$ to $\gamma_a^x$, for $x = 1, 2, 3$, also connects the remaining pairs of states. Finally, if $\det(O) = -1$, the transformation $O$ corresponds to application of the transposition in the standard basis of $\mathbb{C}^2$ followed by application of some unitary operation $U$ [33]. Repeating the same arguments as before we recover (1).

Finally, if vectors from the set $\{n_a^x\}$ span two dimensional space then then the same argument can be repeated using operators $L, O$ acting only in this space (this happens, in particular, if $n = 2$). Importantly, in this case additional transposition is not necessary.

**Remark.** Certification of overlaps between pure states in general does not allow for their self-testing in higher-dimensional systems. This is e.g. due to the existence of unitary inequivalent sets of SIC-POVMs for $d = 3$ [34] and MUBs for $d = 4$ [22] (even if we allow for complex conjugation).

The following theorem shows that the above self-testing argument allows for some level of imperfections present in the observed statistics.

**Theorem 3** (Robust self-testing of qubit systems - qualitative statement). Consider the same structure of target qubit states and measurements as in Theorem 2. Assume that experimental qubit states states $\tilde{\gamma}_a^x$ and measurements $\tilde{M}_b^y$ generate statistics $\tilde{p}(b|a,x,y) = \text{tr}(\tilde{\gamma}_a^x \tilde{M}_b^y)$ such that $|\tilde{p}(b|a,x,y) - \text{tr}(\gamma_a^x M_b^y)| \leq \varepsilon$, for all $a,b = 1, 2$ and $x,y \in [n]$. Then, there exist $\varepsilon_0$ such that for $\varepsilon \leq \varepsilon_0$ there exist a qubit unitary $U$ such that
\[
\frac{1}{2n} \sum_{a,x} \text{tr}(U(\tilde{\gamma}_a^x)^{(T)} U^\dagger \tilde{\gamma}_a^x) \geq 1 - f(\varepsilon),
\]
\[
\frac{1}{2n} \sum_{b,y} \text{tr}(U(\tilde{M}_b^y)^{(T)} U^\dagger \tilde{M}_b^y) \geq 1 - g(\varepsilon),
\]
where $(\cdot)^{(T)}$ is the transposition with respect to a fixed basis in $\mathbb{C}^2$ that may have to be applied to all experimental states and measurements at the same time. Moreover, functions $f, g : [0, \varepsilon_0] \rightarrow \mathbb{R}^+$ depend solely on the target states and measurements and, for small $\varepsilon$, have the asymptotics $f(\varepsilon) \propto \varepsilon$, $g(\varepsilon) \propto \varepsilon$.

In the above result we have used fidelity $F(\rho, \sigma) = \text{tr}(\rho \sigma)$ to indicate the closeness between rotated experimental states and target pure states (and analogously for measurement operators), following existing literature [22]. In Appendix C we give a formal version of the above result and its proof. Moreover, we present there robustness bounds expressed in terms of the trace distance and its analogue for measurements [36]. We remark that the functions $f, g$ become unbounded once Bloch vectors of target qubit states become singular, i.e. once the target states are close to being aligned in a space of smaller dimension. We stress that we use a stronger notion of robust self-testing compared to the one commonly used in
the prepare-and-measure scenario \cite{22,25}. Specifically, we allow only unitary operations (and possible transposition) as opposed to arbitrary channels to be applied to the experimental states in order to approximate the target states as well as possible.

Here is a short outline of the proof. First, we compute the dimension \( k \) of the subspace of \( \mathbb{R}^3 \) spanned by Bloch vectors of all target states. We then chose \( k \) target states whose Bloch vectors are linearly independent. The robustness argument follows form considering Cholesky factorisations of Gram matrices of these vectors and their experimental counterparts, denoted by \( \Gamma \) and \( \tilde{\Gamma} \) respectively. We then apply Theorem 3 (tailored to the qubit scenario) to bound \( \| \Gamma - \tilde{\Gamma} \|_F \) and utilize results of \cite{37} to gauge how much the Cholesky decompositions of \( \Gamma \) and \( \tilde{\Gamma} \) differ in the Frobenious norm. This can be directly connected to the average fidelity between the selected target and experimental states. The robustness for the remaining target states follows from the fact that they can be decomposed (as operators) using the initially chosen \( k \) target states and the identity.

**Examples.** We now apply the quantitative formulation of Theorem 3 to lower-bound average fidelities for different configurations of target quantum states as a function of the allowed error \( \varepsilon \). On Figure 2 we present results for eigenstates of \( n = 2 \) and \( n = 3 \) Pauli matrices (i.e. states forming \( n = 2 \) and \( n = 3 \) qubit MUBs), and states belonging to two biased projective measurements satisfying

\[
\text{tr}(\rho_{a|x}^2 \rho_{a|x}^2) = \frac{1 + \epsilon}{2}, \quad a = 1, 2, \quad \epsilon \in [0, 1].
\]

For \( n = 2 \) MUBs we compare our results with \cite{22} that aimed at self-testing of qubit MUBs. The results of Ref. \cite{22} give the upper bound on average fidelity equal 0.75 for the deviation of \( \varepsilon \approx 0.1 \) in the figure of merit. In our scheme this happens for \( \varepsilon \approx 0.033 \) as shown on Fig. 2.

To test the versatility of our scheme, we also applied it to \( n = 3 \) MUBs, trine and tetrahedral configurations of qubit states. Quantitative results concerning these examples are listed in Table I while detailed derivations are given in the Appendix \cite{22}. For trine and tetrahedral configurations the robustness is obtained via methods, described in Appendix \cite{37} based on \cite{35}. For cases other than two MUBs we cannot make any comparison with the existing literature since, to our best knowledge, these cases have not been studied previously in the literature.

**Shared randomness.** Throughout the article we assumed that preparation and measurement devices are uncorrelated. However, in the presence of shared randomness Alice and Bob share a random variable \( \lambda \) that can be used decide which states and measurements they are going to implement in a given round of the experiment. The most general statistics that can be generated in such a scenario can be expressed as

\[
p(b|a, x, y) = \int d\lambda p(\lambda) \text{tr}(\rho_{a|x}^\lambda M_{b|y}^\lambda),
\]

where \( p(\lambda) \) denotes the probability distribution of \( \lambda \).

The presence of shared randomness makes our techniques inapplicable. The easiest way to see it is to consider the following simple example of \( n = d = 2 \), one bit of shared randomness \( \lambda \in \{1, 2\} \), and \( \rho_{a|x}^{1, 2} = |a\rangle\langle a| \), \( M_{b|y}^{1, 2} = |b\rangle\langle b| \). This clearly satisfies the requirement on \( p(a|a, x, x) = 1 \). Now, Alice and Bob’s devices can decide to “flip” their preparations and measurement operators whenever \( x = 2, y = 2 \) and \( \lambda = 2 \) (note that \( \lambda \) can be distributed in arbitrary way). This procedure does not affect the correlations \( p(a|a, x, y = x) \), but it can be used to set \( p(a|1, 2) \) to arbitrary value.

We believe that in the presence of shared randomness and the bound on the dimension, the usual notion of self-testing has to be reconsidered. Additionally, we believe that in the presence of shared randomness, the usual notion of self-testing in the SDI setting has to be reconsidered. Specifically, for any quantum realisation giving the statistics \( p(b|a, x, y) = \text{tr}(\rho_{a|x}^\lambda M_{b|y}^\lambda) \), one can always consider a strategy in which with probability \( p(\lambda) \) Alice prepares states \( \rho_{a|x}^\lambda = U_\lambda \rho_{a|x} U_\lambda^\dagger \) and Bob implements measurements \( M_{b|y}^\lambda = U_\lambda M_{b|y} U_\lambda^\dagger \), where \( U_\lambda \) is some ar-

\begin{table}[h]
\centering
\begin{tabular}{|l|c|c|}
\hline
Configuration & \( \varepsilon_0 \) & \( C \) \\
\hline
2 MUBs & \( \approx 0.062 \) & \( \frac{3}{7} + \sqrt{2} \) \\
3 MUBs & \( \approx 0.030 \) & \( 6 \) \\
Biased bases & \( \frac{4 - 3\alpha - \sqrt{1 - 4\alpha}}{18} \) & \( \frac{1}{2} + \frac{1}{\sqrt{2}} \sqrt{1 - \alpha} \) \\
Trine & \( \approx 0.058 \) & \( \frac{19}{10} \) \\
Tetrahedron & \( \approx 0.037 \) & \( 10 \) \\
\hline
\end{tabular}
\caption{Results of quantitative variant of Theorem 3 applied to different configurations of target quantum states. The threshold \( \varepsilon_0 \) sets the maximal noise level which is tolerated by our scheme. The constant \( C \) is defined via the relation \( f(\varepsilon) \approx C \varepsilon \), where \( 1 - f \) is the lower bound on the average fidelity from Eq. 3.}
\end{table}
bitary unitary transformation. Clearly, such strategy reproduces the original statistics, and makes it impossible to find a single unitary that connects the target and the experimental states or measurements. Moreover, it creates an obstruction to the “naive” notion of self-testing in the SDI framework with shared randomness as in general one cannot hope to certify states and measurements up to a unitary transformations. Note in the standard Bell scenario we not not have such a problem as shared randomness can be always explained by auxiliary standard Bell scenario we not have such a problem as shared randomness can be always explained by auxiliary

intermediate states to our scheme. Namely, for \( a \neq a', x \neq x' \) we introduce additional state \( \sigma_z \). Let \( \tilde{p}(b|z, y) \) denote the experimentally observed statistics, corresponding to inputs \( z, y \) and outcome \( b \). In the ideal scenario in which experimental statistics satisfy assumptions of Theorem 1 with \( z = 0 \), assume additionally that \( \tilde{p}(a|z, x) + \tilde{p}(a'|z, x) = 1 + \sqrt{p(a'|x, a, x')} \). In Appendix A we prove that under the above assumption for all \( \lambda \) we have \( \text{tr}(\tilde{\sigma}_a^x(\lambda)\tilde{\sigma}_{a'}^x(\lambda)) = \text{tr}(\sigma_a^x\sigma_{a'}^x) \). Since in the ideal case overlaps between preparation states do not depend on \( \lambda \) and match the target value, our modified certification scheme works also in the presence of shared randomness. We postpone the discussion of the non-ideal case as to further work.

Discussion. We have presented a systematic analytical scheme for noise-resilient certification of overlaps between arbitrary configurations of pure quantum states and rank-1 projective measurements in the prepare-and-measure scenario. For qubits our scheme can be used to robustly self-test general ensembles of pure quantum states and the corresponding projective measurements. We believe that these findings pave the way towards systematic certification of general quantum systems in the semi-device-independent paradigm. This is supported by the concrete qubit results from Table I and by the universality of our protocol for certifying overlaps of quantum states in arbitrary dimension.

There is a number of interesting open questions that require further study. First, under what conditions for \( d > 2 \) our certification scheme for overlaps can be used for self-testing in the prepare-and-measure scenario (i.e. identify the states up to unitary transformation and a possible transposition)? Second, can our certification scheme be formulated as a game which score is linear in the observed statistics and is maximised by states and measurements satisfying assumptions of Theorem 1? We believe that enforcing such a linear structure would also improve the robustness of our protocol.

Another way to improve the robustness is to establish better bounds on the difference of Gram matrices of experimental and target states (for example by utilising the bounds from \([39]\)). Finally, it is interesting to combine our method with recent findings relating state discrimination games and resource theories of measurements \([40, 41]\) to give analytical construction of SDI criteria for non-projective character of all extremal measurements. Note added. See also a related work \([42]\).

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Appendix

Here we provide technical details that were omitted in the main part of the article. First, in Appendix A we prove Theorem 1. Second, in Appendix B we prove statements regarding the saturation of bounds derived in that theorem. Later, in Appendix C we formulate and prove a quantitative version of Theorem 3 which concerns robustness of our self-testing protocol expressed in terms of average fidelities. We also prove there Theorem 4 that gives analogous results expressed in trace distance. In Appendix D we give explicit derivations relevant for examples presented in the main text. In Appendix E we give proofs of two auxiliary Lemmas needed in the proof of the technical version of Theorem 3. Finally, in Appendix F we prove technical results regarding the modified version of our certification scheme tailored to the scenario involving shared randomness.

Appendix A: Robustness of the certification scheme for overlaps

**Theorem 1** (Robust SDI certification of overlaps). Consider pure target qudit preparation states \( \sigma_a^x \) and target projective measurements \( M^y \), where \( a \in [d] \) and \( x, y \in [n] \). Assume that \( \sigma_a^x = M_a^x \) for all \( a, x \) and furthermore that experimental states \( \tilde{\sigma}_a^x \) and measurements \( \tilde{M}^y \) act on Hilbert space of dimension at most \( d \) and generate statistics \( \tilde{p}(b|a, x, y) = \text{tr}(\tilde{\sigma}_a^x\tilde{M}_b^y) \) such that \( \tilde{p}(b|a, x, y) - \text{tr}(\sigma_a^xM_b^y) ) \leq \varepsilon \), for all \( a, b, x, y \). Then, input states \( \tilde{\sigma}_a^x \) are almost pure...
in the sense that

$$\text{for all } x \sum_{a=1}^{d} \| \tilde{\varrho}_a^x \| \geq d(1 - 2\varepsilon), \quad (A1)$$

measurements $\tilde{M}^x$ is almost projective in the sense that

$$\text{for all } y \sum_{b=1}^{d} \| \tilde{M}^y_b \| \geq d(1 - \varepsilon), \quad (A2)$$

and for all $x \neq x'$, $a \neq a'$, $y \neq y'$, and $b \neq b'$, we have

$$|\text{tr}(\tilde{\varrho}_a^x \tilde{\varrho}_a^{x'}) - \text{tr}(\tilde{\varrho}_a^x \tilde{\varrho}_a^{x'})| \leq \varepsilon + \sqrt{2\varepsilon + d^2\varepsilon^2}, \quad (A3)$$

$$|\text{tr}(\tilde{M}^y_b \tilde{M}^{y'}_b) - \text{tr}(\tilde{M}^y_b \tilde{M}^{y'}_b)| \leq \varepsilon + (1 + d\varepsilon) \sqrt{2\varepsilon + d^2\varepsilon^2}. \quad (A4)$$

Proof. We start with a straightforward proof of Eq. (A2). Since $\|	ilde{M}^x_a\| \geq \text{tr}(\tilde{M}^x_a \varrho)$ for any state $\varrho$, the relation $\text{tr}(\tilde{\varrho}_a^x \tilde{\varrho}_a^{x'}) \geq 1 - \varepsilon$, valid for all $a, x$ implies $\|	ilde{M}^x_a\| \geq 1 - \varepsilon$, for all $a, x$, and hence for all $x$ we have $\sum_{a=1}^{d} \|	ilde{M}^x_a\| \geq d - d\varepsilon$.

To prove Eq. (A1), that bounds on the norms of experimental states, we fix a setting $x$ and use a decomposition

$$\tilde{M}^x_a = \lambda_a \langle \phi_a | \phi_a \rangle + \text{Rest}_a, \quad (A5)$$

where $\lambda_a$ is the largest eigenvalue of $\tilde{M}^x_a$, $|\phi_a \rangle \langle \phi_a |$ is the corresponding eigenvector and, $\text{Rest}_a$ is a positive-semi-definite operator satisfying $\langle \phi_a | \text{Rest}_a | \phi_a \rangle = 0$. Using the fact that observed statistics are $\varepsilon$ close to target ones we get

$$1 - \varepsilon \leq \text{tr}(\tilde{\varrho}_a^x \tilde{M}^x_a) = \lambda_a \langle \phi_a | \tilde{\varrho}_a^x \rangle | \phi_a \rangle + \text{tr}(\tilde{\varrho}_a^x \text{Rest}_a) \leq \| \tilde{\varrho}_a^x \| + \text{tr}(\text{Rest}_a). \quad (A6)$$

By taking the sum over $a$ we obtain $\sum_{a=1}^{d} \| \tilde{\varrho}_a^x \| \geq d(1 - \varepsilon) - \sum_{a=1}^{d} \text{tr}(\text{Rest}_a)$. We can now use the identity $d = \sum_{a=1}^{d} \text{tr}(\tilde{M}^x_a)$, which follows form that fact that operators $\tilde{M}^x_a$ form a POVM in $\mathbb{C}^d$. This equality allows us to give establish a bound

$$d = \sum_{a=1}^{d} \lambda_a + \sum_{a=1}^{d} \text{tr}(\text{Rest}_a) \leq d(1 - \varepsilon) + \sum_{a=1}^{d} \text{tr}(\text{Rest}_a), \quad (A7)$$

which is equivalent to $\sum_{a=1}^{d} \text{tr}(\text{Rest}_a) \leq d\varepsilon$. Inserting this to $\sum_{a=1}^{d} \| \tilde{\varrho}_a^x \| \geq d(1 - \varepsilon) - \sum_{a=1}^{d} \text{tr}(\text{Rest}_a)$ we obtain Eq. (A1).

We now proceed to the proof of (A3). We start with the one for the overlaps between preparation states. The proof is given by the following sequence of inequalities which hold for every $a \neq a'$, $x \neq x'$.

$$|\text{tr}(\tilde{\varrho}_a^x \tilde{\varrho}_a^{x'}) - \text{tr}(\tilde{\varrho}_a^x \tilde{\varrho}_a^{x'})| \leq |\text{tr}(\tilde{\varrho}_a^x \tilde{\varrho}_a^{x'}) - \text{tr}(\tilde{M}^x_a \tilde{\varrho}_a^{x'})| + |\text{tr}(\tilde{M}^x_a \tilde{\varrho}_a^{x'}) - \text{tr}(\tilde{M}^x_a \tilde{\varrho}_a^{x'})| \leq \| \tilde{\varrho}_a^x - \tilde{M}^x_a \| + \varepsilon \quad (A8)$$

$$\leq \| \tilde{\varrho}_a^x - \tilde{M}^x_a \|_F + \varepsilon = \sqrt{\text{tr}((\tilde{\varrho}_a^x)^2) + \text{tr}((\tilde{M}^x_a)^2) - 2\text{tr}(\tilde{\varrho}_a^x \tilde{M}^x_a)} + \varepsilon \leq \sqrt{1 + (1 + d^2\varepsilon^2) - 2(1 - \varepsilon)} = \varepsilon + \sqrt{2\varepsilon + d^2\varepsilon^2}. \quad (A9)$$

All of the above inequalities are pretty straightforward apart from $\text{tr}((\tilde{M}^x_a)^2) \leq 1 + d^2\varepsilon^2$ that we prove below. For this we again use the partial spectral decomposition form Eq. (A4) (without writing the superscript $x$ as above) which implies

$$\text{tr}((\tilde{M}^x_a)^2) = \lambda_a^2 + \text{tr}(\text{Rest}_a^2) \leq 1 + (\text{tr}(\text{Rest}_a))^2 \leq 1 + d^2\varepsilon^2. \quad (A10)$$

The proof for the overlaps of POVM effects is very similar to the one for states with the only difference being the following inequality

$$|\text{tr}(\tilde{M}^x_a \tilde{M}^{x'}_b) - \text{tr}(\tilde{M}^x_a \tilde{M}^{x'}_b)| \leq (1 + d\varepsilon) \| \tilde{\varrho}_a^x - \tilde{M}^x_a \| \quad (A11)$$

that is used in the second step in the proof in Eq. (A7). One can easily verify the validity of this inequality by writing once more the decomposition $\tilde{M}^x_a = \lambda_a |\phi_{a'} \rangle \langle \phi_{a'} | + \text{Rest}_{a'}$ and remembering that $\text{tr}(\text{Rest}_a) \leq d\varepsilon$. \hfill $\square$
Appendix B: Explicit form of states and measurements saturating the bounds in Theorem 1

We start by giving an example of four states and two qubit measurements \((n = 2, d = 2)\), for which the bound on the deviation of the overlaps scales like \(\sqrt{\epsilon}\). Their explicit form is given below

\[
\begin{align*}
\varrho_1^1 & = |0\rangle\langle 0|, \quad |0\rangle = \sqrt{1-\epsilon}|0\rangle + \sqrt{\epsilon}|1\rangle, \quad \varrho_1^2 = |+\rangle\langle +|,
\end{align*}
\]

where \(|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\), and as required by our scheme \(\varrho_2^x = 1 - \varrho_1^x\), \(x = 1, 2\) and \(M_a^z = \varrho_a^x\), for all \(x, a\). Let the experimental states and measurements be the following

\[
\begin{align*}
\bar{\varrho}_1^1 & = |0\rangle\langle 0|, \quad \bar{\varrho}_2^1 = |1\rangle\langle 1|, \quad \bar{\varrho}_2^2 = |+\rangle\langle +|, \quad \bar{\varrho}_2^2 = |-\rangle\langle -|,
\end{align*}
\]

\[
\begin{align*}
M_1^1 & = |0\rangle\langle 0|, \quad M_1^2 = |+\rangle\langle +|, \quad |+\rangle = \sqrt{1-\epsilon}|+\rangle + \sqrt{\epsilon}|+\rangle.
\end{align*}
\]

First, we need to show that the experimental statistics is deviated from the target one by at most \(\epsilon\), i.e. \(|\text{tr}(\bar{\varrho}_a^1 \bar{\varrho}_a^2) - \text{tr}(\varrho_a^1 \varrho_a^2)| \leq \epsilon, \forall a, b, x, y\). Since \(\bar{\varrho}_1^1 + \bar{\varrho}_2^1 = 1\) for both \(x = 1, 2\), it is sufficient to consider the cases of \(a = 1, b = 1\). Calculating the statistics we can see that \(\text{tr}(\bar{\varrho}_1^1 \bar{\varrho}_1^2) = \text{tr}(\bar{\varrho}_2^2 \bar{\varrho}_2^2) = 1 - \epsilon\), and \(\text{tr}(\bar{\varrho}_1^1 \bar{\varrho}_1^2) = \text{tr}(\bar{\varrho}_2^1 \bar{\varrho}_2^1) = \frac{1}{2} + \sqrt{\epsilon - \epsilon^2}\) and the latter is just the same as the target probability, \(\text{tr}(\varrho_1^1 \varrho_1^2)\). Finally, calculation of the overlap between the states yields

\[
|\text{tr}(\bar{\varrho}_1^1 \varrho_1^2) - \text{tr}(\bar{\varrho}_1^1 \varrho_1^2)| = \sqrt{\epsilon - \epsilon^2},
\]

which confirms the scaling of the first order of \(\sqrt{\epsilon}\).

Now let us show that the bounds from Eq. \((A3)\) are tight in the first order of \(d\). We still consider the case of \(n = 2\), but now we consider arbitrary \(d\). Let us consider the following POVM

\[
\begin{align*}
M_1 & = |1\rangle\langle 1| + \epsilon(d-1)|+\rangle\langle +|, \quad M_a = (|a\rangle - \delta|+\rangle)(\langle a| - \delta|+\rangle) \quad a = 2, 3, \ldots, d,
\end{align*}
\]

where \(\delta = \frac{1}{\sqrt{d-1}} + \frac{\sqrt{d}}{\sqrt{d-1}} - \epsilon\). The computational basis of \(C^d\) and \(|+\rangle = \frac{1}{\sqrt{d}} \sum_{a=2}^d |a\rangle\) is the "maximally coherent" state in the subspace spanned by \(\{|i\rangle\}_{i=2}^d\). In the proof of Theorem 1 the quantity \(|\text{tr}(\tilde{\varrho}_a^x \tilde{\varrho}_a^y) - \text{tr}(\varrho_a^x \varrho_a^y)|\) is upper-bounded by \(\epsilon + \|\tilde{\varrho}_a^x - M_a^x\|\), for which there exist a state \(\tilde{\varrho}_a^x\) and an effect \(\hat{M}_a^x\) reaching the bound. Now if we take \(\hat{M}_a^x\) to be the POVM just introduced, and \(\tilde{\varrho}_a^x = |1\rangle\langle 1|\), \(\tilde{\varrho}_a^x = M_a^x\), the conditions of the Theorem 1 will be satisfied and the resulting bound will be \(d\epsilon\).

Appendix C: Quantitative statement of the robust self-testing

In this part we first formulate Theorem 4 in which we present our robustness of our self-testing scheme in terms of trace distance and operator norm for the case of measurements. Then, we give a quantitative statement of Theorem 3 that concerns robustness of our self-testing scheme in terms of average fidelities. We then proceed with proofs of both results.

In what follows we will need the following definition.

**Definition 1.** Let \(\{\mathbf{n}_i\}_{i=1}^n\) be a set of \(n\) vectors in \(\mathbb{R}^d\). Matrix \(\Gamma \in \mathbb{R}^{n \times n}\) is called Gram matrix of the set \(\{\mathbf{n}_i\}_{i=1}^n\), if its elements are given by \(\Gamma_{i,j} = \mathbf{n}_i \cdot \mathbf{n}_j, i, j \in [n]\).

**Theorem 4 (Robust self-testing for qubits via trace distance and operator norm).** Consider pure target qubit prepa-ration states \(\varrho_a^x\) and target projective measurements \(M_y\), where \(a = 1, 2\) and \(x, y \in [n]\). Assume that \(\varrho_a^x = M_x^y\) for all \(a, x\) and furthermore that experimental states \(\tilde{\varrho}_a^x\) and measurements \(\hat{M}_a^x\) act on Hilbert space of dimension at most \(d\) and generate statistics \(\hat{p}(b|a, x, y) = \text{tr}(\tilde{\varrho}_a^x \hat{M}_b^x)\) such that \(|\hat{p}(b|a, x, y) - \text{tr}(\varrho_a^x \hat{M}_b^x)| \leq \epsilon, \forall a, b, x, y\).

Let \(k \in \{2, 3\}\) be the cardinality of the maximal set of linearly independent Bloch vectors of states \(\varrho_a^1\). Fix a set \(S \subset [n]\) of \(k\) linearly independent vectors \(\{\mathbf{n}_1^x\}_{x \in S}\), construct their Gram matrix \(\Gamma_S\), and let \(L_S\) be a Cholesky factor

\[
\begin{align*}
\|\sigma - \varrho\|_1 = \frac{1}{2} \|\sigma - \varrho\|_1 = \frac{1}{2} \text{tr}(\sqrt{\varrho^T(\sigma - \varrho)^T(\sigma - \varrho)}) \quad \text{and passes a neat opera-}
\end{align*}
\]

1 Recall that the trace distance is defined via \(d_1(\sigma, \varrho) = \frac{1}{2} \|\sigma - \varrho\|_1 = \frac{1}{2} \text{tr}(\sqrt{\varrho^T(\sigma - \varrho)^T(\sigma - \varrho)})\).
of $\Gamma_S$ (i.e. $\Gamma_S = L_S L_S^T$ and $L_S$ is lower triangular). For every $x \in [n] \setminus S$ and both $a = 1, 2$ let $\mathbf{c}_S^a$, denote the coefficients of decomposition of $\mathbf{n}_S^a$ as a linear combination of $\{\mathbf{n}_S^1\}_{x \in S}$. Finally, let us define three auxiliary functions

$$
F_k(\varepsilon) := \sqrt{\varepsilon} \sqrt{4k(k-1)} \frac{1 + 2\sqrt{\varepsilon} + \frac{k + 3}{k - 1} \varepsilon}{k - 1},
$$

$$
O_k(\varepsilon) := 2((k - 1)\sqrt{\varepsilon} + (k + 1)\varepsilon),
$$

$$
E_{S,k}(\varepsilon) := \frac{1}{2\sqrt{2}} \frac{||\Gamma_S^{-1}|| F_k(\varepsilon)}{\sqrt{1 - ||\Gamma_S^{-1}|| O_k(\varepsilon)}} \min \left[ \frac{||\Gamma_S||}{||\Gamma_S||_F}, \frac{||L_S||}{\sqrt{k}} \right]. \tag{C1}
$$

Then, here is a region of $\varepsilon \in [0, \varepsilon_0]$ determined by

$$
||\Gamma_S^{-1}|| O_k(\varepsilon) \leq 1, \tag{C2}
$$

for which there exist a qubit unitary matrix $U$ such that

$$
\frac{1}{k} \sum_{x \in S} d_{tr}(U(\tilde{\varrho}_a^x)^{(T)} U^\dagger, \varrho_1^x) \leq E_{S,k}(\varepsilon), \tag{C3a}
$$

$$
\frac{1}{k} \sum_{x \in S} d_{tr}(U(\tilde{\varrho}_a^x)^{(T)} U^\dagger, \varrho_2^x) \leq E_{S,k}(\varepsilon) + 2\sqrt{\varepsilon}, \tag{C3b}
$$

$$
d_{tr}(U(\tilde{\varrho}_a^x)^{(T)} U^\dagger, \varrho_0^x) \leq \sqrt{k}\mathbf{c}_S^{a,x} | E_{S,k}(\varepsilon) + \frac{\sqrt{k}}{2} \left( \mathbf{c}_S^{a,x} + \sqrt{k} \right) \frac{||\Gamma_S^{-1}|| O_k(\varepsilon)}{1 - ||\Gamma_S^{-1}|| O_k(\varepsilon)}, \text{ for } x \notin S, a = 1, 2, \tag{C3c}
$$

$$
\frac{1}{k} \sum_{y(x) \in S} \left| \left| U(\tilde{\mathbf{M}}_1^x)^{(T)} U^\dagger - M_1^x \right| \right| \leq E_{S,k}(\varepsilon) + \sqrt{\varepsilon}, \tag{C3d}
$$

$$
\left| \left| U(\tilde{\mathbf{M}}_1^y)^{(T)} U^\dagger - M_1^y \right| \right| \leq d_{tr}(U(\tilde{\varrho}_1^y)^{(T)} U^\dagger, \varrho_1^y) + \sqrt{\varepsilon}, \text{ for } y \notin S, \tag{C3e}
$$

where $($(T)$ is the transposition (with respect a fixed basis in $\mathbb{C}^2$) that may have to be applied to all experimental states and measurements simultaneously.

The reason for such a formulation of the Theorem lays in the proof techniques used by us. Namely, we use results on the stability of the Cholesky factorization in the derivation of our bounds. Since result employed by us (Ref. [37]) is valid for positive-definite matrices we need we cannot apply it to the Gram matrix of all of the vectors $\mathbf{n}_a^x$ due to their linear dependence. As a result, our bounds depend on the particular choice of the set $S$ of states whose Bloch vectors are linearly independent. In what follows, without the loss of generality we take $S = \{1, 2\}$ for $k = 2$ and $S = \{1, 2, 3\}$ for $k = 3$ in the proof. In practice, however, one should consider all subsets of states that give non-singular Gram matrices having in mind a specific application.

Outline of the proof. In what follows we will consider a particular subset $\{\mathbf{n}_S^1\}_{x \in S}$ of $k$ linearly independent Bloch vectors. For simplicity we will omit the subscript $S$ whenever possible. The main idea of the proof is to use a Cholesky factors of $k \times k$ the Gram matrices $\Gamma$ and $\tilde{\Gamma}$ of target $(\{\mathbf{n}_S^1\}_{x \in S})$ and and experimental $(\{\tilde{\mathbf{n}}_S^1\}_{x \in S})$ Bloch vectors respectively. We then make use of the result of Ref. [37] on the stability of Cholesky factorization which states that if $\Gamma$ and $\tilde{\Gamma}$ are close to each other, so are their Cholesky factors $L$ and $\tilde{L}$. Specifically, this result, which we quote bellow (see Theorem [Sun 1991]), sets an upper bound on the Frobenious of $\Delta L = L - \tilde{L}$ in terms of the Frobenious norm of the perturbation $\Delta \Gamma = \tilde{\Gamma} - \Gamma$. The Frobenious norm of the perturbation $\Delta L$ can be connected to the trace distance between states $\varrho_1^x$ and the rotated states $\tilde{\varrho}_1^x$ in the selected subset $S$. On the other hand, the bound on $||\Delta \Gamma||_F$ can be estimated from our assumption: $|p(b|a,x,y) - \tilde{p}(b|a,x,y)| \leq \varepsilon$. This is essentially the content of Theorem [1] but here we prove improved qubit stability bounds in Lemma [1] which lead to strong estimates for the norms of $\Delta \Gamma$ in Lemma [2] bellow. Combining all these results produces bounds in Eq. (C3a). In the next part of the proof we determine the trace distance between states $\varrho_2^x$ and $\tilde{\varrho}_2^x$ for $x \in S$ based solely on the fact that $\varrho_2^x = I - \varrho_1^x$ and $\tilde{\varrho}_2^x$ are close to $I - \tilde{\varrho}_1^x$. This gives the bounds in Eq. (C3b). For states $x \notin S$ we use the fact that they can be decomposed in the basis of the states in $S$. Since this linear decomposition can be different for target and experimental states, we use the result on stability of linear systems (see Theorem [Higham 2002], which we also quote below). The bounds for the states $x \notin S$ are given by Eq. (C3c). Finally, we connect the bounds for the distance between the target and experimental measurements and the distance between the corresponding states resulting in Eq. (C3d) and (C3e).

**Theorem 3** (Quantitative formulation of robust self-testing for qubits). Consider pure target qubit preparation states $\varrho_a^x$ and target projective measurements $\mathbf{M}^y$, where $a = 1, 2$ and $x, y \in [n]$. Assume that $\varrho_a^x = M_a^x$ for all $a, x$ and...
then there is a unique Cholesky factorization of its Cholesky factorization. If (Sun 1991 - Stability of Cholesky factorisation)

Before we proceed we state two theorems from the literature that need in our proof. First, we repeat the statement of Theorem 1.4 from Ref. [37] for real-valued matrices. Second, we state a result concerning stability of systems of linear equation, which we borrow from Ref. [45] (Theorem 7.2). We changed the notation used in these papers, furthermore that experimental states $\tilde{\rho}_x$ and measurements $\tilde{M}_y$ act on Hilbert space of dimension at most $d$ and generate statistics $\tilde{p}(b; a, x, y) = tr(\tilde{\rho}_x^y \tilde{M}_y^b)$ such that $|\tilde{p}(b; a, x, y) - \text{tr}(\tilde{\rho}_x^y \tilde{M}_y^b)| \leq \varepsilon$, for all $a, b, x, y$.

Let $k \in \{2, 3\}$ be the cardinality of the maximal set of linearly independent vectors $\{\tilde{\rho}_x^y\}_{x \in S}$, construct their Gram matrix $\Gamma_S$, and let $L_S$ be a Cholesky factor of $\Gamma_S$ (i.e. $\Gamma_S = L_S L_S^T$ and $L_S$ is lower triangular). For every $x \in [n] \setminus S$ and both $a, 1, 2$ let $c_x^{z, 2}$ denote the coefficients of decomposition of $\tilde{\rho}_x^y$ as a linear combination of $\{\tilde{\rho}_x^y\}_{x \in S}$. Finally, let us define three auxiliary functions

\[
F_k(\varepsilon) := \sqrt{\varepsilon} \sqrt{4k(1-k)} \sqrt{1 + 2\sqrt{\varepsilon} + \frac{k+3}{k-1} \varepsilon},
\]

\[
O_k(\varepsilon) := 2((k-1)\sqrt{\varepsilon} + (k+1)\varepsilon),
\]

\[
E_{S,k}(\varepsilon) := \frac{1}{2\sqrt{2}} \frac{\|\Gamma_S^{-1}\| F_k(\varepsilon)}{\sqrt{1 - \|\Gamma_S^{-1}\| O_k(\varepsilon)}} \min \left[ \frac{\|\Gamma_S\|}{\|\Gamma_S\|_F} \frac{\|L_S\|}{\sqrt{k}} \right].
\]

Then, here is a region of $\varepsilon \in [0, \varepsilon_0]$ determined by

\[
\|\Gamma_S^{-1}\| O_k(\varepsilon) \leq 1,
\]

for which there exist a qubit unitary matrix $U$ such that

\[
\frac{1}{k} \sum_{x \in S} \text{tr}(U(\tilde{\rho}_x^y)^{(T)} U^\dagger \tilde{\rho}_x^y) \geq 1 - \frac{\varepsilon(1-2\varepsilon)}{(1-\varepsilon)^2} - E_{S,k}(\varepsilon)^2,
\]

\[
\frac{1}{k} \sum_{x \in S} \text{tr}(U(\tilde{\rho}_x^y)^{(T)} U^\dagger \tilde{\rho}_x^y) \geq 1 - \frac{\varepsilon(1-2\varepsilon)}{(1-\varepsilon)^2} - (E_{S,k}(\varepsilon) + 2\sqrt{\varepsilon})^2,
\]

\[
\text{tr}(U(\tilde{\rho}_a^x)^{(T)} U^\dagger \tilde{\rho}_a^x) \geq 1 - \frac{\varepsilon(1-2\varepsilon)}{(1-\varepsilon)^2} - \left(\text{tr}(U(\tilde{\rho}_a^x)^{(T)} U^\dagger, \tilde{\rho}_a^x)\right)^2, \text{ for } x \notin S, a = 1, 2,
\]

\[
\frac{1}{k} \sum_{y \in S} \text{tr}(U(\tilde{M}_y^x)^{(T)} U^\dagger \tilde{M}_y^x) \geq 1 - \frac{5}{2} \varepsilon - \left(\sqrt{2}E_{S,k}(\varepsilon) + \sqrt{\varepsilon}\right)^2,
\]

\[
\text{tr}(U(\tilde{M}_y^x)^{(T)} U^\dagger \tilde{M}_y^x) \geq 1 - \varepsilon - \left(\text{tr}(U(\tilde{M}_y^x)^{(T)} U^\dagger, \tilde{M}_y^x) + \sqrt{\varepsilon}\right)^2, \text{ for } y \notin S,
\]

where $(\cdot)^{(T)}$ is the transposition (with respect a fixed basis in $C^2$) that may have to be applied to all experimental states and measurements simultaneously. Note that in formulas (C6c) and (C3e) we have used trace distance $\text{d}_t(U(\tilde{\rho}_a^x)^{(T)} U^\dagger, \tilde{\rho}_a^x)$ in order to simplify the resulting formulas. The bound on this quantity is given in Eq. (C8).

Remark. Results of Theorem 3 are obtained using a similar reasoning to that given in the outline of the proof of Theorem 3. However, the proof steps have supplemented via bounds connecting fidelity to the trace distance (for states) and operator norm (for measurement operators). The proof of Theorem 3 is given in the end of this part of the Appendix.

Before we proceed we state two theorems from the literature that need in our proof. First, we repeat the statement of the Theorem 1.4 from Ref. [37] for real-valued matrices. Second, we state a result concerning stability of systems of linear equation, which we borrow from Ref. [45] (Theorem 7.2). We changed the notation used in these papers, making it to the one used in our paper.

Theorem (Sun 1991 - Stability of Cholesky factorisation). Let $\Gamma$ be an $k \times k$ positive definite matrix and $\Gamma = LL^T$ its Cholesky factorization. If $\Delta \Gamma$ is an $k \times k$ symmetric matrix satisfying

\[
\|\Gamma^{-1}\| \|\Delta \Gamma\| \leq 1,
\]

then there is a unique Cholesky factorization

\[
\Gamma + \Delta \Gamma = (L + \Delta L)(L + \Delta L)^T,
\]

and

\[
\|\Delta L\|_F \leq \frac{\|\Gamma^{-1}\| \|\Delta \Gamma\|_F}{\sqrt{2(1 - \|\Gamma^{-1}\| \|\Delta \Gamma\|_F)}} \min \left[ \frac{\|L\|_F \|\Gamma\|_F}{\|\Gamma\|_F}, \|L\| \right].
\]
Remark. This theorem dates back to 1991, and, of course there have been attempts to improve this result. However, the recent review [40] on this topic suggests that the bound given in the Theorem above is the most appropriate in our case (Remark 3.2, Ref. [47]).

Theorem (Higham 2002 - Stability of systems of linear equations). Let \( c \) be a solution of a system of linear equations \( \Gamma c = g \), where \( g \in \mathbb{R}^k \) and \( \Gamma \in \text{Mat}_{k \times k}(\mathbb{R}) \). Let now \( \bar{c} \) be a solution to \( (\Gamma + \Delta \Gamma)\bar{c} = g + \Delta g \), where \( \Delta \Gamma \in \text{Mat}_{k \times k}(\mathbb{R}) \), \( \Delta g \in \mathbb{R}^k \). Assume that there exists \( \delta' > 0 \) such that \( \| \Delta \Gamma \| \leq \delta' \| E \| \) and \( \| \Delta g \| \leq \delta' \| f \| \) (for some \( E \in \text{Mat}_{k \times k}(\mathbb{R}) \), \( f \in \mathbb{R}^k \)), and that \( \delta' \| \Gamma^{-1} \| \| E \| \leq 1 \). Then, we have

\[
\frac{|c - \bar{c}|}{|c|} \leq \frac{\delta'}{1 - \delta' \| \Gamma^{-1} \| \| E \|} \left( \frac{\| \Gamma^{-1} \| \| f \|}{|c|} + \frac{\| \Gamma^{-1} \| \| E \|}{\| f \|} \right).
\] (C9)

Lemma 1. Under the conditions of Theorem 7, qubit states and measurements \( \{ \varrho^x_a \}_{a,x} \), \( \{ M^y \}_{y} \) and \( \{ \tilde{\varrho}^x_a \}_{a,x} \), \( \{ \tilde{M}^y \}_{y} \) satisfy

\[
\| \tilde{\varrho}^x_a \| \geq \frac{1 - \varepsilon}{1 + \varepsilon}, \quad \forall a, x,
\]

\[
\| \tilde{\varrho}^x_a \| \geq \frac{1 - \varepsilon}{1 + \varepsilon}, \quad \forall a, x,
\]

\[
|\text{tr}(\tilde{\varrho}^x_a \tilde{\varrho}^x_{a'}') - \text{tr}(\tilde{\varrho}^x_a \tilde{\varrho}^x_{a'}')| \leq \varepsilon + \sqrt{\varepsilon},
\]

\[
|\text{tr}(\tilde{M}^y_a \tilde{M}^y_{a'}') - \text{tr}(M^y_a M^y_{a'}')| \leq \varepsilon + (1 + \varepsilon)\sqrt{\varepsilon},
\]

\( \forall x \neq x', a \neq a' \) and \( \forall y \neq y', b \neq b' \) respectively, and \( \varepsilon \leq 1/3 \).

Lemma 2. Let \( \Gamma \) be a Gram matrix of Bloch vectors of target states \( \{ \varrho^x \}_{x \in S} \). Likewise, let \( \tilde{\Gamma} \) be a Gram matrix of Bloch vectors of experimental states \( \{ \tilde{\varrho}^x \}_{x \in S} \). Let \( |p(b,a,x,y) - \tilde{p}(b,a,x,y)| \leq \varepsilon \) for all \( b,a,x,y \) and let \( k = |S| \) be the cardinality of the set \( S \). Then, we have the following bounds on norms of \( \Delta \Gamma = \tilde{\Gamma} - \Gamma \)

\[
\| \Delta \Gamma \|_F \leq F_k(\varepsilon),
\]

\[
\| \Delta \Gamma \| \leq O_k(\varepsilon),
\] (C10)

where

\[
F_k(\varepsilon) = \sqrt{\varepsilon} \sqrt{4k(k-1)} \sqrt{1 + 2\sqrt{\varepsilon} + \frac{k+3}{k-1} \varepsilon},
\]

\[
O_k(\varepsilon) = 2((k-1)\sqrt{\varepsilon} + (k+1)\varepsilon).
\]

Proof of Theorem 4. Let \( \tilde{\Gamma} \) be the Gram matrix of Bloch vectors \( \{ \tilde{\varrho}^x \}_{x \in S} \) of the experimental states for \( x \in S \). Let us for now assume that the Cholesky factorization \( \Gamma = \tilde{\Gamma} \tilde{T} \) exists and let \( \Delta \Gamma = \tilde{\Gamma} - \Gamma \).

We start our first part of the proof regarding the states \( x \in S, a = 1 \) by connecting the square of the norm \( \| \Delta \Gamma \|_F \) with trace distance between the states \( \{ \varrho^x \}_{x \in S} \) and \( \{ \tilde{\varrho}^x \}_{x \in S} \). From proof of Theorem 2 it follows that the Bloch vectors \( \{ \varrho^x \}_{x \in S} \) of the target states and the vectors \( \{ \tilde{\varrho}^x \}_{x \in S} \) transpose of which are rows of \( L \) are connected via an orthogonal transformation, which we denote as \( O \), i.e. \( \tilde{L} = O \tilde{\Gamma} \), \( x \in S \). Similarly, for the Bloch vectors \( \{ \varrho^x \}_{x \in S} \) of the experimental states and the vectors \( \{ \varrho^x \}_{x \in S} \) that form \( \tilde{L} \) there exists an orthogonal transformation \( O \), such that \( \tilde{L} = O \tilde{\Gamma} \), \( x \in S \). Let us define states \( \tilde{x} = \frac{1}{2}(1 + \tilde{\Gamma} \cdot \sigma) \), and \( \varrho^x = \frac{1}{2}(1 + \Gamma \cdot \sigma) \), \( x \in S \). We know that there exist unitary transformations \( V \) and \( \tilde{V} \) such that \( \Gamma = V(\varrho^x)(\Gamma)^T V^\dagger \), and \( \tilde{\Gamma} = \tilde{V}(\tilde{\varrho}^x)(\tilde{\Gamma})^T \tilde{V}^\dagger \) for \( x \in S \) (the optional transposition \( (\cdot)^T \) is reserved for the cases det\( (O) = -1 \) and det\( (\tilde{O}) = -1 \)). We have the following sequence of equalities valid for \( x \in S \)

\[
d_{\text{tr}}(\tilde{x}', \tilde{x}) = d_{\text{tr}}(\tilde{V}(\tilde{\varrho}^x)(\tilde{\Gamma})^T \tilde{V}^\dagger, V(\varrho^x)(\Gamma)^T V^\dagger) = d_{\text{tr}}(V^\dagger \tilde{V}(\tilde{\varrho}^x)(\tilde{\Gamma})^T \tilde{V}^\dagger V, (\varrho^x)(\Gamma)^T) = d_{\text{tr}}(U(\varrho^x)(\Gamma)^T U^\dagger, \varrho^x),
\] (C11)

where we used the invariance of trace distance under unitary evolution and transposition, and also denoted the resulting unitary \( V\tilde{V} \) as \( U \). It is clear that one transposition in the final formula in (C11) is enough as the case det\( (O) = \text{det}(\tilde{O}) = -1 \) is equivalent to having det\( (\tilde{O}) = \text{det}(O)1 \) and changing \( U \) to \( U^T \). We need to show now is that this unitary \( U \) satisfies the claim of the Theorem 3 for the states \( x \in S \). For qubits trace distance can be expressed directly via Euclidean distance between Bloch vectors and therefore

\[
d_{\text{tr}}(\tilde{x}', x) = \frac{1}{2} || \tilde{\Gamma} - \Gamma ||_F.
\] (C12)

Using this and Eq. (C11) it is straightforward to derive the following upper bound

\[
\frac{1}{k} \sum_{x=1}^{k} d_{\text{tr}}(U(\varrho^x)(\Gamma)^T U^\dagger, \varrho^x) \leq \frac{1}{2\sqrt{k}} \| \Delta \Gamma \|_F.
\] (C13)
We now use Theorem [Sun 1991] (Ref. 37) to upper-bound $\| \Delta L \|_F$. Specifically, we apply it to the Gram matrix of the Bloch vectors of states $\{ \vec{\varrho}_x \}_{x \in S}$. We have $|L|_F = \sqrt{k}$, since the target states are assumed to be pure. The direct substitution of the bound in Eq. (C5) into Eq. (C13) gives the bound in Eq. (C3a) and also the condition in Eq. (C3), when the Theorem 3 applies. In the beginning of the proof we assumed that the Cholesky factorization $\tilde{\Gamma} = LL^T$ exists. The condition in Eq. (C2) gives the sufficient condition for this to hold. We conclude this part of the proof by noting the Eq. (C6a) follows from application of the reasoning given below Eq. (C27) to Eq. (C13).

In the second part of the proof let us derive upper bounds on the trace distances between the states corresponding to $x \in S$ and $a = 2$. As we will see those can be connected to the bounds for the states with $x \in S$ and $a = 1$. Indeed, we can write the following for every $x \in S$

$$2 d_{tr}(U \vec{\varrho}_x^* U^\dagger, \vec{\varrho}_x^*) = \| \vec{\varrho}_x^* - U \vec{\varrho}_x^* U^\dagger \|_1 \leq \| 1 - \vec{\varrho}_x^* - U(1 - \vec{\varrho}_x^*) U^\dagger \|_1 + \| U(1 - \vec{\varrho}_x^*) U^\dagger \|_1$$

$$\leq \| \vec{\varrho}_x^* - U \vec{\varrho}_x^* U^\dagger \|_1 + \| 1 - \vec{\varrho}_x^* + \tilde{M}_x \|_1 = 2 d_{tr}(U \vec{\varrho}_x^* U^\dagger, \vec{\varrho}_x^*) + \sum_{a=1,2} \| \vec{\varrho}_a^* - \tilde{M}_a \|_1.$$  

Exactly the same reasoning can be applied to upper bound the trace distance $d_{tr}(U \vec{\varrho}_x^* U^\dagger, \vec{\varrho}_x^*)$, in which case the transposition will propagate to $d_{tr}(U (\vec{\varrho}_x^*)^T U^\dagger, \vec{\varrho}_x^*)$ but would not affect the term $\sum_{a=1,2} \| \vec{\varrho}_a^* - \tilde{M}_a \|_1$ (as we can take $(\tilde{M}_a)^T$).

To finish the calculations we need to upper-bound the second summand in Eq. (C14). We do it by writing

$$\| \vec{\varrho}_a^* - \tilde{M}_a \|_1 \leq 2 \| \vec{\varrho}_a^* - M_a \|_1 \leq 2 \sqrt{\varepsilon}, \forall a, x,$$  

where the last inequality is proven in Lemma 1 (see Eq. (F8)). From here, it is easy to obtain the bound in Eq. (C3b). (The reason why we do not simply apply the same reasoning to the states corresponding to $a = 2$ and $x \in S$ as for the states with $a = 1$ is because we want the isometry $U$ to be the same for all of the states.)

In the third part of the proof we derive the bounds for the preparations states corresponding to $x \notin S$ and both $a = 1, 2$. We start by reminding ourselves that the set of states $\{ \vec{\varrho}_x \}_{x \in S}$ is assumed to be tomographically complete. Is is equivalent to the assumption that the vectors $\{ F_x \}_{x \in S}$ defined above are linearly independent and span $\mathbb{R}^k$ for $k = 3$, or the considered subspace for $k = 2$. The condition of the Theorem 3 (also stated in Eq. (C7)) ensures that the same holds for the vectors $\{ F_x \}_{x \in S}$. If so, let us expand the Bloch vectors of the states $\vec{\varrho}_x^*$ and $U \vec{\varrho}_x^* U^\dagger$, $x' \notin S$ in terms of $\{ F_x \}_{x \in S}$ and $\{ F_x \}_{x \in S}$ respectively. Let us denote the coefficients of these linear expansions as $\{ c_{x,x'} \}_{x \in S}$ and $\{ \tilde{c}_{x,x'} \}_{x \in S}$ respectively. These coefficients will, of course, depend on $x'$ and $a'$ as well as on the choice of the set $S$. However, for the simplicity of the derivations we are going omit the subscripts $x'$ and $a'$ until we present the final result. We also remind the reader that we assumed without loss of generality that $S = \{ 1, 2, 3 \}$ (or $S = \{ 1, 2 \}$ for $k = 2$).

It is clear that the coefficients $\{ c_x \}_{x \in S}$ and $\{ \tilde{c}_x \}_{x \in S}$ satisfy the following respective systems of linear equations

$$\Gamma c = g, \quad \tilde{\Gamma} \tilde{c} = \tilde{g},$$  

where $c = (c_1, c_2, c_3)$, $g = (2tr(\vec{\varrho}_x^* \vec{\varrho}_x) - 1, 2tr(\vec{\varrho}_x^* \vec{\varrho}_x) - 1, 2tr(\vec{\varrho}_x^* \vec{\varrho}_x) - 1)$ and analogously $\tilde{c} = (\tilde{c}_1, \tilde{c}_2, \tilde{c}_3)$, $\tilde{g} = (2tr(\tilde{\varrho}_x^* \tilde{\varrho}_x) - 1, 2tr(\tilde{\varrho}_x^* \tilde{\varrho}_x) - 1, 2tr(\tilde{\varrho}_x^* \tilde{\varrho}_x) - 1)$ whenever the cardinality $k$ of the set $S$ is 3. For $k = 2$, $c, \tilde{c}, g, \tilde{g} \in \mathbb{R}^2$ and their definition is analogous. We again omitted the subscripts $a', x'$ for the vectors $g$ and $\tilde{g}$ for simplicity. The matrices $\Gamma$ and $\tilde{\Gamma}$ are still the moment matrices for the states $x \in S$, $a = 1$.

In complete analogy to Eq. (C12) we can write

$$d_{tr}(U (\vec{\varrho}_x^*)^T U^\dagger, \vec{\varrho}_x^*) = \frac{1}{2} \sum_{x \in S} (\tilde{c}_x - c_x) I^F.$$

We then can upper-bound the latter norm as follows

$$\left| \sum_{x \in S} (\tilde{c}_x - c_x) I^F \right| \leq \left| \sum_{x \in S} c_x (I^F - I) \right| + \left| \sum_{x \in S} (\tilde{c}_x - c_x) I^F \right| \leq |c| \| \Delta L \|_F + \sum_{x \in S} |\tilde{c}_x - c_x| \| I^F \| F.$$  

In the equation above we used the following relation

$$\left| \sum_{x \in S} c_x (I^F - I) \right| = \sqrt{\sum_{i=1}^{3} \left( \sum_{x \in S} c_x (I^F - I)^2 \right)} \leq \sqrt{\sum_{i=1}^{3} \sum_{x \in S} (\tilde{I}^F - I^F)^2} = |c| \| \Delta L \|_F.$$  

Also, since the norms $\| I^F \|$ can be upper-bounded by 1 for all $x$, the resulting upper bound can be simplified further to be $|c| \| \Delta L \|_F + \sum_{x \in S} |\tilde{c}_x - c_x|$.  

To estimate the deviation $|c - \bar{c}|$ we apply Theorem [Higham 2002] by taking $\Delta \Gamma = \tilde{\Gamma} - \Gamma$ and $\Delta g = \tilde{g} - g$. The bound on the operator norm $\|\Delta \Gamma\|$ is given by Lemma [4]. At the same time $|\Delta g| = 2\sqrt{\sum_{x \in S} (\text{tr}(\tilde{g}_a^x \rho_1^x) - \text{tr}(\tilde{g}^x_\alpha \tilde{\rho}_1^x))^2} \leq 2\sqrt{k}(\sqrt{2} + \varepsilon)$. If we take $\delta' = 2((k - 1)\sqrt{2} + (k + 1)\varepsilon)$, some matrix $E$ with $\|E\| = 1$, vector $f$ such that $|f| = \frac{\sqrt{k}}{k - 1}$, we satisfy the conditions of the Theorem [Higham 2002] and get the following bound

$$|c - \bar{c}| \leq \left(\frac{1}{k} + \frac{\sqrt{k}}{k - 1}\right) \frac{\|\Gamma^{-1}\| \|\Delta \Gamma\|}{1 - \|\Gamma^{-1}\| \|\Delta \Gamma\|},$$  

(C19)

As the final step we need to connect the bound in Eq. (C17) with the one in Eq. (C19) by the relation between 1-norm and the Euclidean norm in $\mathbb{R}^k$, which effectively adds a factor of $\sqrt{k}$ to the bound in Eq. (C19). Combining everything together we obtain the following

$$d_{tr}(U(\tilde{g}_a^x)^{(T)}U, \tilde{g}_a^x) \leq \frac{1}{2} |c| \|\Delta L\|_F + \frac{\sqrt{k}}{2} \left(\frac{1}{k} + \frac{\sqrt{k}}{k - 1}\right) \frac{\|\Gamma^{-1}\| \|\Delta \Gamma\|}{1 - \|\Gamma^{-1}\| \|\Delta \Gamma\|}, \quad x' \notin S, a' = 1, 2. \quad (C20)$$

The above bound is given in Eq. (C3c) in terms of the quantity $E_{S,k}(\varepsilon)$ (Eq. (C11)) by taking $\|\Delta L\|_F = 2\sqrt{k}E_{S,k}(\varepsilon)$ and with all the necessary subscripts. Again, using the relation in Eq. (C29) we can derive bounds on the fidelity between the states $\tilde{g}_a^x$ and $\tilde{g}_b^x$ for $x \notin S$.

In the fourth, final, part of the proof we derive the bounds for the measurements. We do it by connecting the distance between the experimental measurements and the distance between the corresponding states. Indeed, we can write the following

$$\left\| U(\tilde{M}_1^x)^{(T)}U - M_1^x \right\| \leq \left\| U(\tilde{g}_1^x)^{(T)}U - \tilde{g}_1^x \right\| + \left\| \tilde{g}_1^x - M_1^x \right\|, \quad \forall y, \quad (C21)$$

where we used the triangle inequality and the invariance of the norm $\left\| \tilde{g}_1^x - M_1^x \right\|$ under unitary transformations. Remembering that $\left\| \tilde{g}_1^x - M_1^x \right\| \leq \varepsilon$ (Lemma [1], Eq. (F8)) and $\|U(\tilde{g}_1^x)^{(T)}U - \tilde{g}_1^x\| = d_{tr}(U(\tilde{g}_1^x)^{(T)}U, \tilde{g}_1^x)$ produces the bounds in Eqs. (C3d, C3e).

Finally, we proceed to the proof of Theorem [4] which gives a quantitative robustness analysis expressed in terms of average fidelity.

Proof of Theorem [4]. Let us first state a useful identity between Frobenious distance and fidelity, valid for arbitrary pure states $\varrho$ and Hermitian operator $X$

$$\|X - \varrho\|_F^2 = 1 + \text{tr}(X^2) - 2\text{tr}(X \varrho).$$  

(C22)

We follow exactly the steps that were given in the proof of Theorem [4]. We assume that the reader is familiar with the notation introduced there. First, in order to derive the bound from Eq. (C6a) we repeat the reasoning preceding Eq. (C11). Analogously to the race distance discussed there we use the invariance of the fidelity under unitary transformations and transposition which gives us all $x \in S = [k]$

$$\text{tr}(\tilde{\tau}^x \tau^x) = \text{tr}(U(\tilde{g}_1^x)^{(T)}U, \tilde{g}_1^x), \quad (C23)$$

where $U = V^\dagger \tilde{V}$. Using the above formula and standard algebra involving Pauli matrices we obtain

$$\frac{1}{k} \sum_{x=1}^k \text{tr}(U(\tilde{g}_1^x)^{(T)}U, \tilde{g}_1^x) = \frac{1}{2} + \frac{1}{2k} \sum_{x=1}^k |F|^2 - \sum_{x=1}^k \text{tr}(\tilde{F}^x \cdot \tilde{I}^x).$$  

(C24)

On the other hand we have the following identity

$$\|\Delta L\|_F^2 = \sum_{x=1}^k |F|^2 + \sum_{x=1}^k |\tilde{F}|^2 - 2 \sum_{x=1}^k \text{tr}(\tilde{F}^x \cdot \tilde{I}^x),$$  

(C25)

where $|\cdot|$ is a standard Euclidean norm in $\mathbb{R}^3$. Using the identity $|\tilde{F}|^2 = 2\text{tr}((\tilde{g}_1^x)^2) - 1$ and the fact that target states are pure (which implies $|F| = 1$) we obtain

$$\|\Delta L\|_F^2 = 2 \sum_{x=1}^k \text{tr}((\tilde{g}_1^x)^2) - 2 \sum_{x=1}^k \text{tr}(\tilde{F}^x \cdot \tilde{I}^x).$$  

(C26)
Inserting the above to Eq. (C24) and using \( \text{tr}(\tilde{\rho}^x) \geq 1 - \frac{2\varepsilon(1 - 2\varepsilon)}{(1 - \varepsilon)^2} \) (this follows straightforwardly from Lemma 2), we finally obtain

\[
\frac{1}{k} \sum_{x=1}^{k} \text{tr}(U(\tilde{\rho}^x) (T) U^\dagger \tilde{\rho}^x) \geq 1 - \varepsilon(1 - 2\varepsilon) \left( \frac{1 - \varepsilon}{1 - \varepsilon} + \frac{||\Delta L||^2_F}{4k} \right).
\]  

We complete the proof of Eq. (C6a) by again employing, exactly as before, Theorem [Sun 1991] (Ref. [37]) in order to upper-bound \( ||\Delta L||_F \).

Now, to derive Eq. (C6b), which the bounds for the fidelity of states for \( x \in [k] \) and \( a = 2 \), we can use the following inequality which can be derived from Eq. (C22) and from the formula (C22). In particular, Eq. (C6c) is by setting for \( \Delta = \sum_{k=1}^{k} \text{tr}(\tilde{\rho}^x) (T) U^\dagger, \tilde{\rho}^x) \),

\[
\text{tr}(U(\tilde{\rho}^x) (T) U^\dagger \tilde{\rho}^x) \geq 1 - \varepsilon(1 - 2\varepsilon) \left( \frac{1 - \varepsilon}{1 - \varepsilon} + \frac{||\Delta L||^2_F}{2\sqrt{k}} + 2\varepsilon \right). 
\]

From Eqs. (C13 C14) it follows that

\[
\frac{1}{k} \sum_{x=1}^{k} (d_{tr}(\tilde{\rho}^x) (T) U^\dagger, \tilde{\rho}^x)) \leq \frac{1}{k} \sum_{x=1}^{k} (d_{tr}(\tilde{\rho}^x) (T) U^\dagger \tilde{\rho}^x) + 2\sqrt{\varepsilon}) \leq \frac{\Delta L}{4k} + \frac{2\Delta L}{\sqrt{k}} \varepsilon + 4\varepsilon = \left( \frac{\Delta L}{2\sqrt{k}} + 2\varepsilon \right)^2,
\]

which gives the desired bound form Eq. (C6b).

The proof of remaining formulas (C6c), (C6d) and (C6e) is straightforward and follows directly form Eq. (C22). In particular, Eq. (C6a) is by setting for \( X = \tilde{\rho}^x \) and \( \rho = \rho^x \), inequality \( \text{tr}(\tilde{\rho}^x)^2 \geq 1 - \varepsilon(1 - 2\varepsilon) \) and the relation \( ||\sigma - \rho||_F = \varepsilon \text{tr}(\rho^x) M^x ) \), which holds for arbitrary qubits states \( \rho \) and \( \sigma \). The reasoning is completely analogous for Eq. (C6c) where after setting \( X = M^x \) and \( \rho = \rho^x \) it is additionally necessary to use a (simple) lower bound \( \text{tr}(M^x)^2 \geq (1 - \varepsilon)^2 \), which follows from our assumptions of the theorem. Finally, Eq. (C6d) is derived in a matter which is completely analogous to the justification of Eq. (C6b).

\[ \square \]

**Appendix D: Alternative bounds from Procrustes**

**Lemma 3** (Robust self-testing for qubits from Procrustes). Consider pure target qubit preparation states \( \rho^a \) and target projective measurements \( M^a \), where \( a = 1,2 \) and \( x, y \in [n] \). Assume that \( \rho^a = M^a \) for all \( a, x \) and furthermore that experimental states \( \tilde{\rho}^a \) and measurements \( \tilde{M}^a \) act on Hilbert space of dimension at most \( d \) and generate statistics \( p(b|a, x, y) = \text{tr}(\tilde{\rho}^a M^y) \) such that \( \text{tr}(p(b|a, x, y) - \text{tr}(\tilde{\rho}^a M^y)) \leq \varepsilon \), for all \( a, b, x, y \).

Let \( \{\rho_i\}_{i=1}^{m} \) be a subset of \( m \) considered states among \( \rho^a \). Let \( L \) be a matrix whose rows are the Bloch vectors of states \( \rho_i \) and let \( k \in \{2,3\} \) be its rank \( (m \geq k) \). Assume, without loss of generality, that \( k = 2 \) the third component of the Bloch vectors is 0. In that case, truncate \( L \) to the first two columns. Let us define two auxiliary functions

\[
P_m(\varepsilon, L) = \begin{cases} 
L^\dagger || F_m(\varepsilon) \varepsilon + \sqrt{\text{tr}(F_m(\varepsilon) + L^\dagger || F_m(\varepsilon) + L^\dagger || F_m(\varepsilon))} 
\end{cases} 
\]

and

\[
F_m(\varepsilon) = \sqrt{4m(m - 1)\varepsilon \left( 1 + 2\sqrt{\varepsilon} + \frac{m + 3}{m - 1} \right)},
\]

where \( L^\dagger = (LL^T)^{-1} L^T \). There exist a unitary matrix \( U \) such that

\[
\frac{1}{m} \sum_{i=1}^{m} \text{tr}(\rho_i U \tilde{\rho}_i U^\dagger) \geq 1 - \varepsilon(1 - 2\varepsilon) \left( \frac{1 - \varepsilon}{1 - \varepsilon} - \frac{1}{4m} P_m(\varepsilon, L). \right).
\]
In this section we derive alternative bounds for the fidelity between preparation states that follows from the bounds on the so-called orthogonal Procrustes problem [47]. The problem itself can be formulated as follows. Given two sets of vectors $x_1, x_2, \ldots, x_m$ and $y_1, y_2, \ldots, y_m$ in $\mathbb{R}^d$ find an orthogonal transformation $O \in O(d)$ in $\mathbb{R}^d$ that minimizes $\sum_{i=1}^m |x_i - Oy_i|$. This problem has a clear relevance to our task. Indeed, if we take $x_i$ to be the Bloch vectors of the target qubit preparation states and $y_i$ the Bloch vectors of the experimental states, then minimization over $O(3)$ is the same as the problem of finding a unitary transformation that connects those qubit states. In [38] the bounds on Procrustes problem were derived. We give formulation of Theorem 1 from [38] below, where we change the notation according to our problem.

**Theorem** (Arias-Castro et.al. 2020 - A perturbation bound for Procrustes). Given two tall matrices $L$ and $\tilde{L}$ of same size with $L$ having full rank, and set $\delta^2 = \|\tilde{L}L^T - LL^T\|_F$. Then we have

$$\min_{O \in O(k)} \|L - O\tilde{L}\|_F \leq \begin{cases} \|L^\dagger\| \, \delta^2 + \min \left[ \frac{\|L^\dagger\| \, \delta^2}{\sqrt{1 - ||L^\dagger\| \, \delta^2}}, k^4 \delta \right], & \text{if} \|L^\dagger\| \, \delta < 1 \\ \|L^\dagger\| \, \delta^2 + k^4 \delta, & \text{otherwise.} \end{cases} \quad (D4)$$

In the formulation of the above theorem $L^\dagger$ stands for the Moore-Penrose inverse, which can be defined as $L^\dagger = (LL^T)^{-1}L^T$ for tall matrices of full rank.

**Proof of Lemma 2.** Unitizing the results of the Theorem [Arias-Castro et.al. 2020] is rather straightforward. Let $L$ be a matrix which rows are Bloch vectors of all target preparation states $\{\varrho_a^x\}_{a,x}$. Let $\tilde{L}$ in turn be the matrix of Bloch vectors of the experimental states $\{\tilde{\varrho}_a^x\}_{a,x}$. The matrices $LL^T$ and $\tilde{L}\tilde{L}^T$ are then, of course, the full Gram matrices $\Gamma$ and $\tilde{\Gamma}$. By “full” we mean that now we do not select a subset $S$ of linearly independent vectors among the Bloch vectors of $\varrho_a^x$. Instead, $\Gamma$ and $\tilde{\Gamma}$ are formed by all the considered states, which can still be a subset of the $2n$ states ($x \in [n], a \in [2]$). We will be using $m$ as to denote the number of the considered states, and a simple one-indexed set $\{\varrho_i\}_{i=1}^m$ to denote the states themselves. Estimating $\delta^2$ from the formulation of the Theorem [Arias-Castro et.al. 2020] is a direct application of the bound on $\|\Delta \Gamma\|_F$ from Lemma 2 where now instead of $k$ one should put the number $m$ of the considered preparation states.

As for the left-hand side of Eq. (D4), we can write the following

$$\|L - O\tilde{L}\|_F^2 = \text{tr}(LL^T) + \text{tr}(\tilde{L}\tilde{L}^T) - 2\text{tr}(L^T O\tilde{L}) \geq m + m - \frac{4\varepsilon(1 - 2\varepsilon)}{(1 - \varepsilon)^2} - 4 \sum_{i=1}^{m} \text{tr}(\varrho_i U \tilde{\varrho}_i U^\dagger) + 2m \quad (D5)$$

where we use the following identity

$$\text{tr}(L^T O\tilde{L}) = \sum_{i=1}^{m} n_i \cdot O\tilde{n}_i = 2 \sum_{i=1}^{m} \text{tr}(\varrho_i U \tilde{\varrho}_i U^\dagger) - m, \quad (D6)$$

and $U$ is the unitary transformation in $SU(2)$ corresponding to the orthogonal transformation $O$ of the Bloch vectors. The bound on the average fidelity between $m$ target preparation states and the corresponding experimental states is then simply

$$\frac{1}{m} \sum_{i=1}^{m} \text{tr}(\varrho_i U \tilde{\varrho}_i U^\dagger) \geq 1 - \frac{\varepsilon(1 - 2\varepsilon)}{(1 - \varepsilon)^2} - \frac{1}{4m} P_m^2(\varepsilon, L) \quad (D7)$$

where

$$P_m(\varepsilon, L) = \begin{cases} \|L^\dagger\| F_m(\varepsilon) + \min \left[ \frac{\|L^\dagger\| F_m(\varepsilon)}{\sqrt{1 - ||L^\dagger\| \, F_m(\varepsilon)^2}}, \sqrt{\kappa F_m(\varepsilon)} \right], & \text{if} \|L^\dagger\| \, \sqrt{F_m(\varepsilon)} < 1 \\ \|L^\dagger\| F_m(\varepsilon) + \sqrt{\kappa F_m(\varepsilon)} & \text{otherwise,} \end{cases} \quad (D8)$$

and

$$F_m(\varepsilon) = \sqrt{4m(m - 1)\varepsilon \left(1 + 2\sqrt{\varepsilon + \frac{m + 3}{m - 1}\varepsilon}\right)}. \quad (D9)$$

□
Appendix E: Examples

In this section of the Appendix we present the explicit forms of our analytical bounds for the examples given in the main text. The first example concerns \( n = 2, 3 \) MUBs in \( d = 2 \). Since for MUBs \( \text{tr}(\varrho_a \varrho_a') = \frac{1}{2} \), for \( x \neq x', \forall a, a' \), it follows that \( \Gamma \) is an identity matrix in \( \mathbb{R}^n \) \((n \in \{2, 3\})\). Hence, in Theorem 3 we should take \( \|\Gamma_s\| = \|\Gamma_s^{-1}\| = \|L_s\| = 1 \), and \( \|\Gamma\|_F = \sqrt{n} \). The resulting bound is the average between expressions in Eq. (C3a) and Eq. (C3b) with the function \( E_{S,k}(\varepsilon) \) being simply

\[
E_{S,k}(\varepsilon) = \frac{1}{2\sqrt{2n}} \frac{F_k(\varepsilon)}{\sqrt{1 - O_k(\varepsilon)}}.
\] (E1)

The leading linear term is given in Table I for both \( n = 2, 3 \).

The second example is a little less straightforward. From the condition \( \text{tr}(\varrho_1^1 \varrho_2^2) = \frac{1 + \alpha}{2} \), \( \alpha \in (-1, 1) \) we obtain that \( \Gamma = (\frac{1}{\sqrt{1 - \alpha^2}}) \), and hence \( \|\Gamma\| = 1 + |\alpha|, \|\Gamma^{-1}\| = \frac{1}{\sqrt{1 - |\alpha|^2}} \), and \( \|\Gamma\|_F = \sqrt{2 + 2|\alpha|^2} \). The output of the Cholesky factorization is \( L = \left(\frac{1}{\sqrt{1 - \alpha^2}} \right) \), which leads to \( \|L\| = \sqrt{1 + |\alpha|} \). This also determines the minimum in Eq. (C1) to be \( \sqrt{1 + |\alpha|} \). Plugging this values in Eq. (C1) gives

\[
E_{(1,2),2}(\varepsilon) = \frac{1}{4} \sqrt{1 + |\alpha|} F_k(\varepsilon).
\] (E2)

The final bound is again the average of the bounds in Eq. (C3a) and Eq. (C3b). The first order in \( \varepsilon \) for this bound is given in Table I. The applicability of the above bound is determined by the inequality \( 1 - |\alpha| - O_2(\varepsilon) \geq 0 \). The latter condition gives nonempty region \( \varepsilon \in [0, c_0) \) whenever \( |\alpha| > 0 \).

The third example is a trine ensemble of states \((\varrho_1^1, \varrho_2^2, \varrho_3^3)\), with \( \varrho_1^1 = \frac{1}{2} + \frac{1}{2} x \cdot \sigma, x = 1, 2, 3 \), and where \( \varrho_1 = (1, 0, 0), \varrho_2 = (-\frac{1}{2}, \sqrt{\frac{3}{2}}, 0), \) and \( \varrho_3 = (-\frac{1}{2}, -\sqrt{\frac{3}{2}}, 0). \) For this configuration of preparation states the alternative robustness analysis via Procrustes (see Appendix D) gives better bounds. Given the vectors \( \varrho_i, i = 1, 2, 3 \) we can directly compute that \( \|L^\dagger\| = \sqrt{\frac{3}{2}} \). Inserting this value to Lemma 3 produces the results given in Table I.

The fourth example is the tetrahedron, with \( \varrho_1 = (0, 0, 1), \varrho_2 = \left(\frac{\sqrt{3}}{2}, 0, -\frac{1}{2}\right), \varrho_3 = \left(-\frac{\sqrt{3}}{2}, \sqrt{\frac{3}{2}}, -\frac{1}{2}\right), \varrho_4 = \left(-\sqrt{\frac{3}{2}}, -\sqrt{\frac{3}{2}}, 1\right), \) and \( \varrho_1^1 = \frac{1}{2} + \frac{1}{2} x \cdot \sigma, x = 1, 2, 3, 4 \) as before. In this case we also employ the bounds from Procrustes. For the above configuration of states we have that \( \|L^\dagger\| = \sqrt{\frac{3}{2}} \), which leads to the results in Table I.

Appendix F: Proofs of auxiliary results

Proof of Lemma 7 First of all, we improve the bound on the norm of each of the experimental states. From \( \|\tilde{M}_b^x\| \geq 1 - \varepsilon \), for \( d = 2 \) it follows immediately that the second (second largest) eigenvalue of each of the effects \( \tilde{M}_b^x \) cannot exceed \( \varepsilon \). Hence, we can conclude that \( \text{tr}(\tilde{M}_b^x) \leq 1 + \varepsilon, \forall b \geq b \).

Secondly, we can improve the bound on the norm of each of the experimental states. For that let us write the spectral decomposition of each of \( \varrho_a^x = \eta(1 + |\langle \psi|\psi\rangle|) + (1 - \eta)|\langle \psi|\psi\rangle| = \eta 1 + (1 - 2\eta)|\langle \psi|\psi\rangle| \) and the effect \( \tilde{M}_a^x \) as \( \tilde{M}_a^x = \lambda_0|\langle \phi|\phi\rangle| + \lambda_1(1 - |\langle \phi|\phi\rangle|) \), where we assume that \( \lambda_0 \geq \lambda_1 \). We omitted the indices \( x, a \) for \( \eta, \lambda_0, \lambda_1 \) and \( \psi, \phi \) for simplicity. We can assume without loss of generality that \( \eta \geq \frac{1}{2} \), and let us also assume for now that \( |\langle \phi|\psi\rangle|^2 \leq \frac{1}{2} \).

From the condition \( \text{tr}(\tilde{M}_b^x) \geq 1 - \varepsilon \), it then follows that

\[
\eta(\lambda_0 + \lambda_1) + (1 - 2\eta)(\lambda_0|\langle \phi|\psi\rangle|^2 + \lambda_1(1 - |\langle \phi|\psi\rangle|^2)) \geq 1 - \varepsilon,
\] (F1)

from where we can obtain a lower bound on \( \eta \), namely

\[
\eta \geq \frac{1 - \varepsilon - \lambda_1}{\lambda_0 + \lambda_1 - \frac{1}{2} |\langle \phi|\psi\rangle|^2} + \frac{1}{2}.
\] (F2)

The expression on the right-hand side of the above inequality is maximum when \( |\langle \phi|\psi\rangle|^2 = 0 \) and \( \lambda_0 = 1, \lambda_1 = \varepsilon \), which returns the bound \( \|\tilde{M}_b^x\| \geq \frac{1 - \varepsilon}{\lambda_0 - \lambda_1} \).

Now let us return to our assumption \( |\langle \phi|\psi\rangle|^2 \leq \frac{1}{2} \) for which the above bound is valid. We can upper-bound \( \eta \) by 1 in Eq. (F1), which returns nontrivial upper bound on \( |\langle \phi|\psi\rangle|^2 \) that happens to be \( 1 - \frac{1 - \varepsilon}{\lambda_0 - \lambda_1} \). This function is below \( \frac{1}{2} \)
for $\varepsilon \leq \frac{1}{2}$, i.e. for $\varepsilon \leq \frac{1}{2}$ our newly-derived bound on $\|\tilde{\varrho}_a\|$ is valid. The region $\varepsilon \in [0, \frac{1}{2}]$ is significantly larger than the resulting region in which our self-testing argument will be valid, so this assumption does not affect our final results.

Let us now try to improve the bounds for the overlaps. In the proof of Theorem 1 (see Eq. (A7)) we have already established that

$$\text{tr}(\tilde{\varrho}_a \tilde{\varrho}_b) - \text{tr}(\tilde{\varrho}_a \tilde{\varrho}_b) = \varepsilon + \|\tilde{\varrho}_a - \tilde{M}_a\|.$$ \hspace{1cm} (F3)

Let us now refine the bound on $\|\tilde{\varrho}_a - \tilde{M}_a\|$. For simplicity we present this result below for a pair of operators $\varrho = (1 - \eta)\mathbb{1} + (2\eta - 1)\varphi \psi$ and $M = \lambda_1\mathbb{1} + (\lambda_0 - \lambda_1)\phi \psi$, that satisfy the conditions $\text{tr}(\varrho M) \geq 1 - \varepsilon$, and $1 - \varepsilon \leq \lambda_0 \leq 1$, $0 \leq \lambda_1 \leq \varepsilon$. To compute the norm, we look for an eigenvector $|\xi\rangle$, $(\varrho - M)|\xi\rangle = \Lambda|\xi\rangle$ and obtain the following quadratic equation for $\Lambda$

$$\Lambda^2 - \Lambda(1 - \lambda_0 - \lambda_1) + \eta(1 - \eta) - \lambda_0 \lambda_1 - \eta(\lambda_0 - \lambda_1) + (2\eta - 1)(\lambda_0 - \lambda_1)(\phi \psi)^2 = 0.$$ \hspace{1cm} (F4)

The sum of the roots of this equation is equal to $1 - \lambda_0 - \lambda_1$. Since we know that $|1 - \lambda_0 - \lambda_1| \leq \varepsilon$, then either both roots are of the same sign, in which case the largest eigenvalue could only be $\varepsilon$, or they are of the opposite sign. In the latter case it is evident that the absolute values of both roots are maximal whenever the free term in Eq. (F4) is minimal. We then can upper-bound the solutions to Eq. (F4) by lower-bounding the free term using the condition $\text{tr}(\varrho M) \geq 1 - \varepsilon$. Indeed, from $\text{tr}(\varrho M) \geq 1 - \varepsilon$ we infer immediately that

$$\text{tr}(\varrho M) = \lambda_0 - \eta(\lambda_0 - \lambda_1) + (2\eta - 1)(\lambda_0 - \lambda_1)(\phi \psi)^2 \geq 1 - \varepsilon,$$ \hspace{1cm} (F5)

and thus we reduce Eq. (F4) to

$$\Lambda^2 - \Lambda(1 - \lambda_0 - \lambda_1) + \eta(1 - \eta) - \lambda_0 \lambda_1 + \lambda_0 \lambda_1 + 1 - \varepsilon = 0.$$ \hspace{1cm} (F6)

Using the same argument we can set $\eta = 1$, because $\eta(1 - \eta) \geq 0$. The positive root of Eq. (F6) is equal to

$$\Lambda = \frac{1 - \lambda_0 - \lambda_1}{2} + \sqrt{\frac{(1 - \lambda_0 - \lambda_1)^2}{2} - (1 - \lambda_0)(1 - \lambda_1) + \varepsilon}.$$ \hspace{1cm} (F7)

It is easy to check that the above expression does not have any local maxima w.r.t $\lambda_0, \lambda_1$ on the domain $1 - \varepsilon \leq \lambda_0 \leq 1$, $0 \leq \lambda_1 \leq \varepsilon$, whenever $\varepsilon < \frac{1}{2}$, which we assume to be the case. Thus, we conclude that the maximal value of $\Lambda$ corresponds to the boundary of the region of $(\lambda_0, \lambda_1)$. By considering this boundary we find that this maximal value corresponds to the case of $\lambda_0 = 1$ and $\lambda_1 = 0$ which yields $\Lambda = \sqrt{\varepsilon}$. From the above argument we finally conclude that

$$\|\tilde{\varrho}_a - \tilde{M}_a\| \leq \sqrt{\varepsilon}, \forall x \neq x', \forall a,$$ \hspace{1cm} (F8)

which completes the proof for the state overlaps. From Eq. (F8) and $\text{tr}(\tilde{M}_a^2) \leq 1 + \varepsilon$ it is easy to obtain the improved bound on the overlaps between measurement effect.

**Proof of Lemma 3** Let us start by deriving the bound on the Frobenious norm $\|\Delta\Gamma\|_F

$$\|\Delta\Gamma\|_F^2 = \sum_{x=1}^{k}|||\Gamma_{x,x'} - \tilde{\Gamma}_{x,x'}|||^2 \leq \sum_{x \neq x'} \sum_{x \neq x'} \text{tr}(\tilde{\varrho}_a \tilde{\varrho}_b - \text{tr}(\tilde{\varrho}_a \tilde{\varrho}_b)).$$ \hspace{1cm} (F9)

We have already established the bound on $\|\text{tr}(\tilde{\varrho}_a \tilde{\varrho}_b - \text{tr}(\tilde{\varrho}_a \tilde{\varrho}_b))\|$ in Lemma 1. The bound on $(1 - \text{tr}(\tilde{\varrho}_a \tilde{\varrho}_b))^2$ can be obtained from the bound on the norm of each $\tilde{\varrho}_a$. Namely, from the condition $\|\tilde{\varrho}_a\| \geq \frac{1 - \varepsilon}{3}$ we can immediately conclude that

$$1 - \text{tr}(\tilde{\varrho}_a \tilde{\varrho}_b) \leq \frac{2\varepsilon(1 - 2\varepsilon)}{(1 - \varepsilon)^2}.$$ \hspace{1cm} (F10)

From here it is easy to get to the final bound on $\|\Delta\Gamma\|_F^2$, which reads

$$\|\Delta\Gamma\|_F^2 \leq 4k(k - 1)(\varepsilon + \sqrt{\varepsilon})^2 + \frac{16k^2(1 - 2\varepsilon)^2}{(1 - \varepsilon)^4} \leq 4k(k - 1)\varepsilon \left(1 + 2\sqrt{\varepsilon} + \frac{k + 3}{k - 1}\varepsilon\right),$$ \hspace{1cm} (F11)

where we made some approximations to simplify the result.

Now, let us derive the bound on $\|\Delta\Gamma\|$. In principle, we know that $\|\Delta\Gamma\| \leq \|\Delta\Gamma\|_F$, but we can derive better bounds based on the fact that the diagonal entries of $\Delta\Gamma$ are much less than the off-diagonal entries.
First of all, due to the triangle inequality, we can write \( \| \Delta \Gamma \| \leq \| \text{diag}(\Delta \Gamma) \| + \| \text{offdiag}(\Delta \Gamma) \| \), where we split \( \Delta \Gamma \) on diagonal and off-diagonal parts. The first term \( \| \text{diag}(\Delta \Gamma) \| \) can be easily bounded as follows

\[
\| \text{diag}(\Delta \Gamma) \| = 2 \max_{k} (1 - \text{tr}(\rho_i^2))^2 \leq \frac{4 \varepsilon (1 - 2 \varepsilon)}{(1 - \varepsilon)^2} \leq 4 \varepsilon.
\]  

(F12)

As for the off-diagonal part, we give the proof for two cases \( k = 2 \) and \( k = 3 \) separately. For \( k = 2 \), \( \| \text{offdiag}(\Delta \Gamma) \| = 2 |\text{tr}(\rho_1^2) - \text{tr}(\rho_1^2)| \leq 2 \sqrt{\varepsilon} + 2 \varepsilon \), where we used the results of Lemma 1. As for \( k = 3 \), we will need some intermediate result, namely the following relation

\[
\| \mathbf{A} \| \leq \sqrt{\frac{k - 1}{k}} \| \mathbf{A} \|_F,
\]

(F13)

where \( k \) is the size of the matrix \( \mathbf{A} \) with \( \text{tr}(\mathbf{A}) = 0 \). We give a proof of this below.

Let us assume that \( \{\lambda_i\}_{i=1}^{k} \) are the eigenvalues of matrix \( \mathbf{A} \), hence we know that \( \sum_{i=1}^{k} \lambda_i = 0 \). Let \( \lambda_1 \) be the largest eigenvalue, i.e. the norm of \( \mathbf{A} \), if \( \lambda_1 \geq 0 \). If we wish to maximize the Frobenious norm of \( \mathbf{A} \) for fixed \( \lambda_1 \), the following lower-bound has to be satisfied

\[
\| \mathbf{A} \|_F^2 = \lambda_1^2 + \sum_{i=2}^{k} \lambda_i^2 \geq \frac{1}{k - 1} \left( \sum_{i=2}^{k} |\lambda_i| \right)^2 \geq \frac{1}{k - 1} \left( \sum_{i=2}^{k} \lambda_i \right)^2 = \lambda_1^2 \frac{k}{k - 1},
\]

(F14)

which proves the bound. Using the above result we obtain the following bound

\[
\| \text{offdiag}(\Delta \Gamma) \| \leq \sqrt{\frac{2}{3}} \| \text{offdiag}(\Delta \Gamma) \|_F = 2 \sqrt{\frac{2}{3}} \sqrt{\sum_{x \neq x'} |\text{tr}(\rho_1^2) - \text{tr}(\rho_1^2)|^2} \leq 4(\sqrt{\varepsilon} + \varepsilon),
\]

(F15)

which completes out proof.

\[ \square \]

**Appendix G: Shared randomness**

Here we discuss in detail the modification of our SDI certification scheme that allows to certify overlaps between arbitrary pure states even in the presence of shared randomness. The idea is to introduce, for every pair of non-orthogonal states, a suitable intermediate state \([39] \), that enforces fixed overlaps between experimental states in every round of the experiment.

Recall that in our certification scheme we have pure target qudit states \( \rho^a_{x} \) and target projective measurements \( \mathbf{M}^a \), where \( a \in [d] \) and \( x, y \in [n] \). We extend this scheme by introducing additional intermediate target state \( \sigma_z \) for every two pairs of Alice’s input \((x, a)\), \((x', a')\), where \( a \neq a' \) and \( x \neq x' \). The state \( \sigma_z \) is chosen as the unique state satisfying

\[
\text{tr} \left( \sigma_z (\rho^a_{x} + \rho^{a'}_{x'}) \right) = 1 + \text{tr} (\rho^a_{x} \rho^{a'}_{x'})^2.
\]

(G1)

Consider now a general physical realisation of experimental statistics \( \hat{p}(b|x, a, y), \hat{p}(b|z, y) \) via classically correlated preparation and measurements on \( \mathbb{C}^d \)

\[
\hat{p}(b|x, a, y) = \int d\lambda p(\lambda) \text{tr}(\rho^a_{x} (\lambda) \mathbf{M}^a_{y} (\lambda)) ,
\]

(G2)

\[
\hat{p}(b|z, y) = \int d\lambda p(\lambda) \text{tr}(\sigma_z (\lambda) \mathbf{M}^a_{y} (\lambda)) ,
\]

(G3)

where \( x, y \in [n], a, b \in [d] \) and the variable (input) \( z \) labels elements in the set of unordered pairs \( \{ (x, a), (x', a') \} \), where \( x \neq x' \) and \( a \neq a' \). Assume now that the above statistics match exactly the ones required by our scheme and are compatible with (G1) in the sense that

\[
\hat{p}(b|x, a, y) = \text{tr}(\rho^a_{x} \rho^{a'}_{x'}) ,
\]

(G4)

\[
\hat{p}(a|z, x) + \hat{p}(a'|z, x') = 1 + \sqrt{\hat{p}(a'|x, a')}. \quad (G5)
\]


In what follows we prove that if the above constraints are satisfied, then for all \( x \) \( x' \in [a], \ a, \ a' \in [d] \).

\[
\tilde{\sigma}^x_a(\lambda) = \tilde{M}^x_a(\lambda), \quad (G6)
\]

\[
\text{tr}(\tilde{\sigma}^x_a \tilde{\sigma}^{x'}_{a'}) = \text{tr}(\tilde{\sigma}^x_a(\lambda)\tilde{\sigma}^{x'}_{a'}(\lambda)), \quad (G7)
\]

where \( x, x' \in [a], \ a, a' \in [d] \). The above equation means that the overlaps between preparation states (and measurements) do not depend on the value of the shared random variable \( \lambda \).

The proof of Eq. (G6) is straightforward. Namely, form Eq. (G4) it follows that

\[
\int d\lambda p(\lambda) \text{tr} \left( \tilde{\sigma}^x_a(\lambda)\tilde{M}^x_a(\lambda) \right) = 1. \quad (G8)
\]

Since \( \text{tr}(\tilde{\sigma}^x_a(\lambda)\tilde{M}^x_a(\lambda)) \leq 1 \) we get that for all \( \lambda \) we have \( \text{tr}(\tilde{\sigma}^x_a(\lambda)\tilde{M}^x_a(\lambda)) = 1 \). Since this reasoning can be repeated for all \( a \in [d] \) (for the fixed value of \( x \)) and operators \( M^x_a \) form a POVM on \( \mathbb{C}^d \), we finally get (G6).

The proof of Eq. (G7) is more involved and relies on both (G4) and (G5). Specifically, from (G4) and the already established identity \( \tilde{\sigma}^x_a = \tilde{M}^x_a \) it follows that Eq. (G5) is equivalent to

\[
\int d\lambda p(\lambda) \text{tr} \left( \tilde{\sigma}_x(\lambda)\tilde{\sigma}^{x'}_{a'}(\lambda) + \tilde{\sigma}^{x'}_{a'}(\lambda)\tilde{\sigma}_x(\lambda) \right) = 1 + \sqrt{\text{tr}(\tilde{\sigma}^x_a \tilde{\sigma}^{x'}_{a'})}. \quad (G9)
\]

where moreover

\[
\int d\lambda p(\lambda) \text{tr} \left( \tilde{\sigma}^x_a(\lambda)\tilde{\sigma}^{x'}_{a'}(\lambda) \right) = \text{tr}(\tilde{\sigma}^x_a \tilde{\sigma}^{x'}_{a'}). \quad (G10)
\]

Using Bloch representation of qubit states (states \( \tilde{\sigma}^x_a(\lambda), \tilde{\sigma}^{x'}_{a'}(\lambda) \) are pure and hence span a two dimensional subspace of \( \mathbb{C}^d \)) it is straightforward to obtain the bound

\[
\text{tr} \left( \tilde{\sigma}_x(\lambda)\tilde{\sigma}^{x'}_{a'}(\lambda) + \tilde{\sigma}^{x'}_{a'}(\lambda)\tilde{\sigma}_x(\lambda) \right) \leq 1 + \sqrt{\text{tr}(\tilde{\sigma}^x_a \tilde{\sigma}^{x'}_{a'})}. \quad (G11)
\]

After setting \( g(\lambda) = \sqrt{\text{tr}(\tilde{\sigma}^x_a(\lambda)\tilde{\sigma}^{x'}_{a'}(\lambda))} \) and using Eq. (G10) we obtain

\[
\int d\lambda p(\lambda) g(\lambda) \geq \sqrt{\int d\lambda p(\lambda) g(\lambda)^2}. \quad (G12)
\]

Using Cauchy-Schwartz inequality for the left hand side of the above inequality we finally get

\[
\int d\lambda p(\lambda) g(\lambda) = \sqrt{\int d\lambda p(\lambda) g(\lambda)^2}, \quad (G13)
\]

which is equivalent to saying that the variance of the random variable \( g(\lambda) \) vanishes. Therefore, \( g(\lambda) = \alpha \), where \( \alpha \) is some numerical constant. We conclude the proof by noting that from Eq. (G10) it follows that \( \alpha^2 = \text{tr}(\tilde{\sigma}^x_a \tilde{\sigma}^{x'}_{a'}) \) which implies Eq. (G7).

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