

Witnessing measurement incompatibility via communication tasks

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Quantum theory offers measurement incompatibility, that is, the existence of quantum measurements that cannot be carried out simultaneously on single systems. Measurement incompatibility is essential for probing many aspects of quantum correlations and quantum information processing. However, its fundamental and generic link with nonclassical correlations observed in the simplest prepare-and-measure scenario is still untold. In the prepare-and-measure scenario, we uncover that d -dimensional classical systems assisted with shared randomness reproduce all the input-output statistics obtained from any set of d -dimensional compatible quantum measurements. Thus, any quantum advantage in one-way communication tasks with d -dimensional systems witnesses incompatibility of the measurements on the receiver's end in a semi-device-independent way. To witness incompatibility of an arbitrary number of quantum measurements acting on an arbitrary dimension, wherein different measurements have different outcomes, we introduce a class of communication tasks - a general version of random access codes. We provide generic upper bounds on the success metric of these tasks for compatible measurements. These bounds are tight whenever the dimension on which the measurements act is not larger than the number of outcomes of any of the measurements.

I. INTRODUCTION

In the standard quantum theory, a set of quantum measurements is called incompatible if these measurements cannot be performed simultaneously on a single copy of a quantum system [1]. This notion of measurement incompatibility is one of the fundamental features of quantum theory that differentiates quantum mechanics from the formulation of classical physics. Quantum measurement incompatibility is at the root of demonstrating various fundamental quantum aspects ranging from Bell-nonlocality [2, 3], Einstein–Podolsky–Rosen steering [4–6], measurement uncertainty relations [7, 8], quantum contextuality [9, 10], quantum violation of macrorealism [11], to temporal and channel steering [12–14].

Bell inequality violation is the most compelling operational witness of incompatible measurements since it relies only on the input-output statistics of bipartite systems [3, 15, 16]. Further, measurement incompatibility can also be witnessed through Einstein–Podolsky–Rosen steering [4–6, 17]. These protocols, however, rely on entanglement. Only recently, witnessing of quantum measurement incompatibility in the prepare-and-measure scenario based on some state discrimination task [18] has been proposed. It is particularly noteworthy that measurement incompatibility is necessary but not sufficient for Bell inequality violations employing fully untrusted devices [19, 20], whereas incompatibility is shown to be necessary as well as sufficient in steering with one-sided trusted devices [5, 6] and in state discrimination task with fully trusted preparations [21] (also see [22, 23]).

Notwithstanding, the generic link between measure-

ment incompatibility and nonclassical correlations in the simplest prepare-and-measure scenario is still not fully explored. The present article is motivated towards filling this important gap in the relevant literature. Moreover, the results presented here address whether incompatible quantum measurements are necessary for probing quantum advantage in any one-way communication task. Apart from addressing this fundamental question, this work aims to provide an operational witness of incompatibility for any set of quantum measurements of an arbitrary setting - any set of an arbitrary number of measurements acting on an arbitrary (but finite) given dimension wherein different measurements have different arbitrary number of outcomes.

Specifically, we consider the one-way communication scenario consisting of two players, say, Alice (sender) and Bob (receiver). Alice and Bob are given inputs such that each player does not know the input of the other player. Alice, upon receiving her input, sends classical or quantum communication to Bob. Bob, upon receiving his input and the communication sent by Alice, produces the outputs. In such scenario, we show that any quantum advantage in an arbitrary communication task over all possible classical strategies with unlimited shared randomness implies that the quantum measurements performed by Bob to produce the outputs are incompatible. Therefore, any one-way communication task in prepare-and-measure scenario serves as a tool to witness measurement incompatibility in a semi-device independent way. Furthermore, we point out that whenever the figure of merit of any task is a convex function of the input-output statistics, its maximum value in classical communication and quantum communication with compatible measurements are the same.

The result [24], that a pair of quantum measurements is incompatible whenever it provides advantage in random access code task, becomes a corollary of our observation.

Subsequently, we focus on a specific quantum communication task in the prepare-and-measure scenario, namely, Random Access Codes (RAC) [25]. Based on the operational figure of merit of this task, we propose a witness of measurement incompatibility of a set of arbitrary number of quantum measurements having arbitrary number of outcomes acting on arbitrary dimensional state. Specifically, we derive upper bound (or, exact value in specific cases) of the average success probability of RAC assisted with the best classical strategy, or equivalently the best quantum strategy involving compatible measurements by the receiver. Therefore, given any set of quantum measurements, if the average success probability of RAC involving the given measurements by the receiver exceeds the above bound, then we can certify that the given measurements are incompatible. Here, it should be noted that RAC, being one of the fundamental quantum communication protocols, has been implemented in a series of experiments [26–31]. Hence, the results presented in this study can be used as experimental tool to witness measurement incompatibility based on present day technology. Finally, we identify all sets of three incompatible rank-one projective qubit measurements that can be witnessed by RAC. We next proceed by first explaining the definition of measurement incompatibility, followed by detailed analysis and discussions of illustrative results.

II. QUANTUM MEASUREMENT INCOMPATIBILITY

An arbitrary measurement is conceptualized by some Positive Operator-Valued Measure (POVM) defined as $E_y \equiv \{M_{b_y|y}\}_{b_y}$ with $M_{b_y|y} \geq 0$ for all b_y and $\sum_{b_y} M_{b_y|y} = \mathbb{1}$. Here y corresponds to the choice of measurement, and b_y denotes the outcomes of measurement y .

A set of measurements $\{E_y\}_y$ with $y \in [n]$ (here we use the notation $[k] := \{1, \dots, k\}$) is compatible [1] if there exists a parent POVM $\{G_\kappa : G_\kappa > 0 \forall \kappa, \sum_\kappa G_\kappa = \mathbb{1}\}$ and classical post-processing for each y given by $\{P_y(b_y|\kappa)\}$ such that

$$\forall b_y, y, \quad M_{b_y|y} = \sum_\kappa P_y(b_y|\kappa) G_\kappa. \quad (1)$$

Post-processing for each y is defined by $\{P_y(b_y|\kappa)\}$ such that

$$P_y(b_y|\kappa) \geq 0 \quad \forall y, b_y, \kappa; \quad \sum_{b_y} P_y(b_y|\kappa) = 1 \quad \forall y, \kappa. \quad (2)$$

III. INCOMPATIBILITY IS NECESSARY FOR QUANTUM ADVANTAGE IN COMMUNICATION TASKS

Now, we will show that incompatible measurements are necessary for showing quantum advantage in any communication task. Before proceeding, let us briefly describe a generic communication scenario consisting of two players - Alice and Bob. Alice and Bob are given inputs $x \in [l]$ and $y \in [n]$, respectively. Further, initially neither player has any idea about the other player's input. Alice, upon receiving the input x sends a d -dimensional classical or quantum system to Bob. Bob, upon receiving the input y and the message (which is d -dimensional classical or quantum system) sent by Alice, outputs $b_y \in [d_y]$. The outcome of this communication task is determined by the set of probabilities distributions $\{p(b_y|x, y)\}$.

In classical communication, they can use pre-shared randomness λ , and therefore, the any typical probability can be expressed as

$$p(b_y|x, y) = \sum_{m=1}^d \int_\lambda \pi(\lambda) p_a(m|x, \lambda) p_b(b_y|y, m, \lambda) d\lambda. \quad (3)$$

Here $\{p_a(m|x, \lambda)\}, \{p_b(b_y|y, m, \lambda)\}$ are encoding and decoding functions by Alice and Bob, satisfying non-negativity and

$$\sum_m p_a(m|x, \lambda) = \sum_{b_y} p_b(b_y|y, m, \lambda) = 1. \quad (4)$$

While in quantum communication

$$p(b_y|x, y) = \text{Tr}(\rho_x M_{b_y|y}), \quad \rho_x, M_{b_y|y} \in \mathcal{B}(\mathbb{C}^d) \quad (5)$$

Here $\mathcal{B}(\mathbb{C}^d)$ stands for the space of all operators acting on d dimensional complex Hilbert space. Let l, n, d_y be some natural numbers. Given the scenario $x \in [l], y \in [n], b_y \in [d_y]$, we define the set all probabilities obtainable by d -dimensional classical communication

$$\mathcal{C}_d := \{p(b_y|x, y)\} \quad (6)$$

where $p(b_y|x, y)$ is given by (3), and the set of all probabilities in d -dimensional quantum communication

$$\mathcal{Q}_d := \{p(b_y|x, y)\} \quad (7)$$

where $p(b_y|x, y)$ is given by (5). We are interested in another set of probabilities,

$$\mathcal{Q}_d^C := \{p(b_y|x, y)\} \quad (8)$$

where $p(b_y|x, y)$ is given by (5) such that the set of measurements acting on d -dimensional quantum states used by Bob $\{M_{b_y|y}\}$ is compatible according to (1).

Result 1. *Given any scenario,*

$$\mathcal{Q}_d^C \subseteq \mathcal{C}_d, \quad (9)$$

that is, measurement incompatibility is necessary for any advantage over classical communication. However, measurement incompatibility is not sufficient for quantum advantage.

Proof. Consider the case where Bob performs a single POVM measurement $\{G_\kappa\}$, which is the parent POVM of the measurement set $\{M_{b_y|y}\}$. Thanks to the Frenkel-Weiner theorem [32], which implies that the set of input-output probabilities $p(\kappa|x)$ with a single quantum measurement on d -dimensional quantum states can be always be reproduced by a suitable classical d -dimensional communication in the presence of shared randomness. That is, $\forall \rho_x$, there exists classical strategy $\pi(\lambda), p_a(m|x, \lambda), p_b(\kappa|m, \lambda)$ such that

$$\text{Tr}(\rho_x G_\kappa) = \sum_{m=1}^d \int_{\lambda} \pi(\lambda) p_a(m|x, \lambda) p_b(\kappa|m, \lambda) d\lambda. \quad (10)$$

Here note that the scenario considered by Frenkel-Weiner [32] is a bit different since Bob does not receive any input y therein. That is why Bob's output κ depends only on the message m sent by Alice and classical shared randomness λ . On the other hand, Bob receives the message m as well as an input y in the aforementioned communication scenario. Hence, in the communication task, Bob's output b_y depends on m, y and classical shared randomness λ (see Eq.(3)).

Let us now focus on the aforementioned communication scenario and take into account the following decoding function,

$$p_b(b_y|y, m, \lambda) = \sum_{\kappa} P_y(b_y|\kappa) p_b(\kappa|m, \lambda), \quad (11)$$

where $\{P_y(b_y|\kappa)\}$ is the post-processing to obtain $M_{b_y|y}$ from the parent POVM defined in (1). One can check that this is indeed a valid decoding function.

Next, we show that an arbitrary $p(b_y|x, y) \in \mathcal{Q}_d^C$ in the communication scenario can always be reproduced by a suitable classical strategy involving the decoding function (11). An arbitrary $p(b_y|x, y) \in \mathcal{Q}_d^C$ can always be expressed as $p(b_y|x, y) = \text{Tr}(\rho_x M_{b_y|y})$, where $M_{b_y|y}$ satisfies (1). Now, with the help of (10), one can show the following,

$$\begin{aligned} & \text{Tr}(\rho_x M_{b_y|y}) \\ &= \sum_{\kappa} P_y(b_y|\kappa) \text{Tr}(\rho_x G_\kappa) \\ &= \sum_{\kappa} P_y(b_y|\kappa) \left(\sum_m \int_{\lambda} \pi(\lambda) p_a(m|x, \lambda) p_b(\kappa|m, \lambda) d\lambda \right) \\ &= \sum_m \int_{\lambda} \pi(\lambda) p_a(m|x, \lambda) \left(\sum_{\kappa} P_y(b_y|\kappa) p_b(\kappa|m, \lambda) \right) d\lambda \end{aligned}$$

$$= \sum_m \int_{\lambda} \pi(\lambda) p_a(m|x, \lambda) p_b(b_y|y, m, \lambda) d\lambda. \quad (12)$$

Therefore, an arbitrary probability distribution $p(b_y|x, y)$ obtainable from compatible set of measurement can be reproduced by a suitable classical strategy, inferring that $\mathcal{Q}_d^C \subseteq \mathcal{C}_d$.

Since the figure of merit of any communication task is some arbitrary functions of the probabilities $p(b_y|x, y)$, we can infer that any advantage in such tasks over classical communication can be attained only if the set measurements $\{E_y \equiv \{M_{b_y|y}\}_{b_y}\}_y$ is incompatible.

Finally, we note that there exists incompatible qubit measurements such that the probabilities obtained from them for arbitrary quantum states are within \mathcal{C}_2 (see Section IV-A of [33]). This completes the proof. \square

We are often interested in linear functions of $\{p(b_y|x, y)\}$ due to their practical importance in quantum communication complexity tasks [34–36], quantum key distribution [37], quantum randomness generation [38, 39], quantum random access codes [24, 40], oblivious transfer [36, 41] and many other applications. To find the optimum value of any linear function of $\{p(b_y|x, y)\}$, it is sufficient to consider classical strategy without shared randomness (see Lemma 1 in the Appendix A for detailed explanation). As a consequence, all probability distributions $\{p(b_y|x, y)\}$, that are obtained from classical strategy without shared randomness, can always be reproduced by the following quantum strategy. Upon receiving the input x , Alice sends the quantum state ρ_x such that ρ_x is diagonal in some basis. Bob, upon receiving the input y and the state ρ_x , performs a fixed measurement $\{G_\kappa\}$, which is independent of y and nothing but the measurement in that basis, followed by some post-processing depending on y . Therefore, we have another useful result.

Result 2. *The maximum value of any linear function of $\{p(b_y|x, y)\}$ obtained within the two sets \mathcal{C}_d and \mathcal{Q}_d^C is same.*

Above results have profound implications in practice. As a consequence of them we are able to conclude that any arbitrary communication task can serve as a witness of measurement incompatibility. Next, we will propose incompatibility witness for an arbitrary set of measurements for a family of communication tasks, namely, the general version of random access codes [25].

IV. INCOMPATIBILITY WITNESS FOR SETS OF MEASUREMENTS OF ARBITRARY SETTING

Take the most general form of a set of measurements. There are n measurements, defined by $\{M_{b_y|y}\}$ where $y \in [n]$ each of which has different outcomes, say, measurement y has d_y outcomes, that is, $b_y \in [d_y]$, and

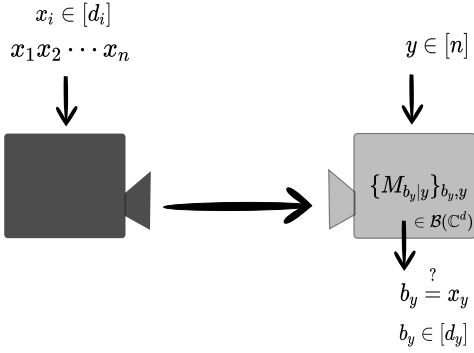


FIG. 1. An unknown measurement set of arbitrary settings, $\{M_{b_y|y}\}_{b_y, y}$, is provided; we only know the dimension (d) on which this set of measurements act. Our task is to certify the incompatibility of this set of measurements. Here, the notation $[k] := \{1, \dots, k\}$ for any natural number k .

these measurement are acting on d -dimensional quantum states (see FIG. 1). In order to witness incompatibility of this set we introduce the most general form of random access codes with Bob having this set of measurements. Alice gets a string of n dits $x = x_1 x_2 \dots x_n$ randomly from the set of all possible strings in which $x_y \in [d_y]$ for all $y \in [n]$. While Alice communicates a d -dimensional classical or quantum system to encode the information about obtained string, the task for Bob is to guess the y -th dit when y is chosen randomly. The figure of merit is the average success probability defined by the following linear function

$$S(n, \vec{d}, d) = \frac{1}{n \prod_y d_y} \sum_{x, y} p(b_y = x_y | x, y) \quad (13)$$

that is fully specified by $n, \vec{d} = (d_1 d_2 \dots d_n)$, and d . Since this (13) is a linear function of $p(b_y | x, y)$, by Result 2, the maximum value over \mathcal{C}_d and \mathcal{Q}_d^C is the same and denoted by $S^C(n, \vec{d}, d)$. Precisely,

$$\begin{aligned} S^C(n, \vec{d}, d) &= \max_{\{p(b_y|x, y)\} \in \mathcal{C}_d} S(n, \vec{d}, d) \\ &= \max_{\{p(b_y|x, y)\} \in \mathcal{Q}_d^C} S(n, \vec{d}, d). \end{aligned} \quad (14)$$

Hence, $S^C(n, \vec{d}, d)$ can be evaluated by maximizing the average success probability either over all classical strategies, or over all quantum strategies involving compatible measurements only.

Whenever a set of measurements in the scenario specified by n, \vec{d}, d gives $S(n, \vec{d}, d) > S^C(n, \vec{d}, d)$ in above-introduced general version of the random access codes, we can conclude that the measurements are incompatible. Hence, in order to witness measurement incompatibility, we need to know $S^C(n, \vec{d}, d)$. Now we present an upper bound on $S^C(n, \vec{d}, d)$ for arbitrary n, \vec{d}, d .

Result 3. The following relation holds true for arbitrary n, \vec{d}, d ,

$$S^C(n, \vec{d}, d) \leq \frac{1}{n} \times \min \left\{ 1 + \sum_{i < j} \frac{d}{d_i d_j}, n - 1 + \frac{d}{\prod_y d_y} \right\}. \quad (15)$$

This upper bound in Eq. (15) is obtained for \mathcal{Q}_d^C , that is, by taking the existence of a parent POVM of the measurements $\{M_{b_y|y}\}_{b_y, y}$ performed by Bob. The proof of this result is presented in the Appendix A. When the outcome of all the measurements are same, which is $d_y = \vec{d}$ for all y , the above bound simplifies to

$$S^C(n, \vec{d}, d) \leq \frac{1}{n} \times \min \left\{ 1 + \frac{n(n-1)d}{2d^2}, n - 1 + \frac{d}{\vec{d}^n} \right\}. \quad (16)$$

Hence, in different types of RAC involving an arbitrary set of quantum measurements by Bob, if the average success probability exceeds the aforementioned upper bounds on S^C , then we can conclude that the measurements by Bob are incompatible.

On the other hand, whenever

$$d \leq \min_y d_y \quad (17)$$

we find out the exact value of $S^C(n, \vec{d}, d)$. Say, k_i is the number of sets among $[d_1], \dots, [d_n]$ such that dit $i \in [d_y]$. For example, consider the random access codes with $n = 4$ and $d_1 = 2, d_2 = 3, d_3 = 4$ and $d_4 = 3$. That is, Alice gets a string of four dits $x = x_1 x_2 x_3 x_4$ randomly, where $x_1 \in [2], x_2 \in [3], x_3 \in [4]$ and $x_4 \in [3]$. In this case, $k_1 = 4, k_2 = 4, k_3 = 3, k_4 = 1$. Also, we denote $d_{\max} = \max_y d_y$.

Result 4. If (17) holds then

$$S^C(n, \vec{d}, d) = \frac{1}{n \prod_y d_y} \sum \left[\left(\prod_{j=1}^{d_{\max}} C_{n_j}^{\alpha_j} \right) \max_{i=1, \dots, d} \{n_i\} \right] \quad (18)$$

with

$$\alpha_j = k_j - \sum_{i=j+1}^{d_{\max}} n_i, \quad C_{n_j}^{\alpha_j} = \frac{\alpha_j (\alpha_j - 1) \dots (\alpha_j - n_j + 1)}{n_j (n_j - 1) \dots 1}$$

and where the summation is taken over all possible integer solutions of the following equation

$$\sum_{i=1}^{d_{\max}} n_i = n \quad (19)$$

such that $n_i \leq k_i$ for all i ,

Note here that (18) is obtained for \mathcal{C}_d by considering the classical strategies. The detailed proof is given in the Appendix B. For a particular case of Result 4 wherein

$d_y = \vec{d} = d$ for all y , the proof is previously given in [40]. Hence, when $d \leq \min_y \vec{d}_y$, the necessary criteria for a set of measurements to be compatible is given by,

$$S(n, \vec{d}, d) \leq S^C(n, \vec{d}, d), \quad (20)$$

where $S^C(n, \vec{d}, d)$ is given by (18).

For $n = 2$, $d_y = \vec{d}$ for all y , and $d \leq \vec{d}$, the expression (18) simplifies to (for details, see the Appendix C)

$$S^C(2, \vec{d}, d) = \frac{1}{2\vec{d}^2} (d + 2d\vec{d} - d^2). \quad (21)$$

And for $n = 3$, $d_y = \vec{d}$ for all y , and $d \leq \vec{d}$, the expression (18) simplifies to (for details, see the Appendix C)

$$S^C(3, \vec{d}, d) = \frac{d}{3\vec{d}^3} (d^2 - 1 + 3\vec{d}(\vec{d} + 1 - d)). \quad (22)$$

The particular case of *Result 3* for $n = 2$ can be found in [24], and moreover, it is shown that any pair of rank-one projective measurements that are incompatible provides advantage in RAC [8]. In order to showcase the generic applicability of *Results 3-4*, we consider an arbitrary set of three rank-one projective qubit measurements, which using the freedom of unitary can be expressed as

$$\begin{aligned} M_{x_1|1} &= (1/2)U[\mathbb{1} + (-1)^{x_1}\sigma_z]U^\dagger \\ M_{x_2|2} &= (1/2)U\left[\mathbb{1} + (-1)^{x_2}\left(\alpha\sigma_z + \sqrt{1-\alpha^2}\sigma_x\right)\right]U^\dagger \\ M_{x_3|3} &= (1/2)U\left[\mathbb{1} + (-1)^{x_3}\left(\beta\sigma_z + \gamma\sqrt{1-\beta^2}\sigma_x \right. \right. \\ &\quad \left. \left. \pm \sqrt{1-\beta^2}\sqrt{1-\gamma^2}\sigma_y\right)\right]U^\dagger \end{aligned} \quad (23)$$

where $x, x_2, x_3 \in [2]$, the variables $\alpha, \beta, \gamma \in [-1, 1]$, and U can be arbitrary unitary operator acting on \mathbb{C}^2 . We obtain the following result.

Result 5. *Any set of three incompatible rank-one projective qubit measurements, except for the sets defined by (23) with*

$$(\alpha, \beta, \gamma) = \{(\pm 1/2, \pm 1/2, -1), (\pm 1/2, \mp 1/2, 1)\}$$

and arbitrary U , yields larger value than $S^C(n = 3, \vec{d} = 2, d = 2) = 3/4$.

This result is proved with the help of numerical optimizations and the proof is put over to Appendix D.

V. CONCLUSION

By characterizing the set of quantum correlations in prepare-and-measure scenarios produced from any set

of compatible measurements, we have shown in this article that incompatible measurements at the receiver's end is necessary for demonstrating quantum advantage in any one-way communication task. Further, based on this result, we have presented a semi-device independent witness of measurement incompatibility invoking generalized random access codes. Interestingly, we have completely characterized the sets of three incompatible projective qubit measurements that can be detected using our proposed witness. It might be noted that some of the results derived in [8, 24] appear as natural corollaries of the results obtained here.

The significance of the result presented here lies in the fact that the classical bound of the success metric of any one-way communication task becomes an upper bound on the metric of the task under compatible set of measurements. Consequently, violating the classical bound of any one-way communication task can be used as a sufficient criteria to witness measurement incompatibility. Further, the present study establishes that measurement incompatibility is the fundamental quantum resource for non-classicality in any one-way communication task or, more generally, in prepare-and-measure scenarios.

Our study opens up the possibilities of several open questions. First of all, deriving more efficient incompatibility witnesses based on different communication tasks is worth for future studies. Secondly, our results may be generalized to propose semi-device witnesses for incompatible quantum channels [42] and quantum instruments [43, 44]. Though we have proved that \mathcal{Q}_d^C is a subset of \mathcal{C}_d for any d , we strongly anticipate that \mathcal{Q}_d^C is in fact a strict subset of \mathcal{C}_d . It needs further investigation to prove this. Finally, proposing operational witnesses for all incompatible extremal POVM [45] is another fundamentally motivated open problem.

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Appendix A: Proof of Result 3

Proof. For a given set of measurements, the maximum average success probability in quantum theory is given by [8]

$$S^C(n, \vec{d}, d) = \frac{1}{n \prod_y d_y} \sum_{x_1 x_2 \dots x_n} \|\chi\|, \quad (\text{A1})$$

where,

$$\chi = M_{x_1|1} + M_{x_2|2} + \dots + M_{x_n|n}. \quad (\text{A2})$$

Here $\|\chi\|$ denotes operator norm of χ , which is nothing but the maximum eigenvalue of the operator χ . An alternative definition of measurement incompatibility, which is equivalent to the standard one (1), is associated with the existence of a parent POVM whose appropriate marginals give rise to all the individual measurements [1]. Precisely,

if the measurements $\{M_{b_y|y}\}$ are compatible then there exists a parent measurement, $G \equiv \{G(b_1, \dots, b_n)\}$, with $\prod_{y=1}^n d_y$ elements from which all the measurement operators can be reconstructed by taking marginals as follows

$$M_{x_y|y} = \sum_{b_1, \dots, b_{y-1}, b_{y+1}, \dots, b_n} G(b_1, \dots, b_{y-1}, x_y, b_{y+1}, \dots, b_n), \quad (\text{A3})$$

where

$$\sum_{b_1, \dots, b_n} G(b_1, \dots, b_{y-1}, b_y, b_{y+1}, \dots, b_n) = \mathbb{1}_{d \times d}. \quad (\text{A4})$$

Let us first expand χ in terms of the parent POVM using (A3),

$$\chi = \sum_{b_2, b_3, \dots, b_n} G(x_1, b_2, b_3, \dots, b_n) + \sum_{b_1, b_3, \dots, b_n} G(b_1, x_2, b_3, \dots, b_n) + \dots + \sum_{b_1, b_2, b_3, \dots, b_{n-1}} G(b_1, b_2, b_3, \dots, b_{n-1}, x_n). \quad (\text{A5})$$

Each term in the above expansion can be split into two terms in the following way

$$\begin{aligned} \chi &= \sum_{b_3, b_4, \dots, b_n} G(x_1, x_2, b_3, b_4, \dots, b_n) + \sum_{\substack{b_2, \dots, b_n \\ b_2 \neq x_2}} G(x_1, b_2, \dots, b_n) \\ &+ \sum_{b_1, b_4, \dots, b_n} G(b_1, x_2, x_3, b_4, \dots, b_n) + \sum_{\substack{b_1, b_3, \dots, b_n \\ b_3 \neq x_3}} G(b_1, x_2, b_3, \dots, b_n) \\ &+ \dots \\ &+ \sum_{b_2, b_3, \dots, b_{n-1}} G(x_1, b_2, b_3, \dots, b_{n-1}, x_n) + \sum_{\substack{b_1, \dots, b_{n-1} \\ b_1 \neq x_1}} G(b_1, \dots, b_{n-1}, x_n). \end{aligned} \quad (\text{A6})$$

In the above Eq. (A6), there are two sums in each line, and there are total n lines. Let us denote the first sum and the second sum in the i^{th} line by \mathcal{S}_1^i and \mathcal{S}_2^i respectively, where $i \in \{1, \dots, n\}$. Hence, Eq. (A6) can be expressed as

$$\chi = \sum_{i=1}^n (\mathcal{S}_1^i + \mathcal{S}_2^i), \quad (\text{A7})$$

where

$$\mathcal{S}_1^i = \sum_{b_1, \dots, b_{i-1}, b_{i+2}, \dots, b_n} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, b_{i+2}, \dots, b_n), \quad (\text{A8})$$

and

$$\mathcal{S}_2^i = \sum_{\substack{b_1, \dots, b_{i-1}, b_{i+1}, \dots, b_n \\ b_{i+1} \neq x_{i+1}}} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_n). \quad (\text{A9})$$

Here the index i is taken to be modulo n . Each $G(\dots)$ in the above sums will be termed as an element.

Let us now make an observation that there is no common element between the \mathcal{S}_2^i and \mathcal{S}_2^{i+1} . The common element between \mathcal{S}_2^i and \mathcal{S}_2^j with $i, j \in \{1, \dots, n\}$ and $j > i + 1$ is

$$\begin{aligned} &\sum_{\substack{b_1, \dots, b_n \\ b_{i+1} \neq x_{i+1} \\ b_{j+1} \neq x_{j+1}}} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \\ &\leq \sum_{\substack{k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \end{aligned} \quad (\text{A10})$$

where the index i, j is taken to be modulo n . Hence, we have

$$\sum_{i=1}^n \mathcal{S}_2^i \leq \sum_{\substack{i, j \in \{1, \dots, n\} \\ j > i+1}} \left(\sum_{\substack{k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right) + \text{other terms with no common element.} \quad (\text{A11})$$

Next, let us focus on \mathcal{S}_1^i . It can be checked that

$$\sum_{i=1}^n \mathcal{S}_1^i = \sum_{i=1}^n \left(\sum_{\substack{k=1 \\ k \neq i, i+1}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, x_{i+1}, b_{i+2}, \dots, b_n) \right). \quad (\text{A12})$$

Replacing \mathcal{S}_2^i and \mathcal{S}_1^i using (A11) and (A12) in (A7), we have

$$\begin{aligned} \chi &\leq \sum_{\substack{i, j \in \{1, \dots, n\} \\ i < j}} \left(\sum_{\substack{k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right) + \text{other terms with no common element} \\ &\leq \sum_{\substack{i, j \in \{1, \dots, n\} \\ i < j}} \left(\sum_{\substack{k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right) + \sum_{b_1, \dots, b_n} G(b_1, \dots, b_n). \end{aligned} \quad (\text{A13})$$

Substituting the above expression into (A1) and employing the triangle inequality for norm, we find that

$$\begin{aligned} S^C(n, \vec{d}, d) &\leq \frac{1}{n \prod_y d_y} \left(\sum_{x_1, \dots, x_n} \sum_{\substack{i, j \in \{1, \dots, n\} \\ i < j}} \left\| \sum_{\substack{k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right\| \right. \\ &\quad \left. + \sum_{x_1, \dots, x_n} \left\| \sum_{b_1, \dots, b_n} G(b_1, \dots, b_n) \right\| \right). \end{aligned} \quad (\text{A14})$$

Due to (A4) the second term of the above expression can be evaluated as

$$\sum_{x_1, \dots, x_n} \left\| \sum_{b_1, \dots, b_n} G(b_1, \dots, b_n) \right\| = \sum_{x_1, \dots, x_n} \left\| \mathbb{1}_{d \times d} \right\| = \prod_{y=1}^n d_y. \quad (\text{A15})$$

Next, Consider the first term in (A14) given by,

$$\sum_{x_1, \dots, x_n} \sum_{\substack{i, j \in \{1, \dots, n\} \\ i < j}} \left\| \sum_{\substack{k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right\| = \sum_{\substack{i, j \in \{1, \dots, n\} \\ i < j}} \beta_{i, j} \quad (\text{A16})$$

where

$$\begin{aligned} \beta_{i, j} &= \sum_{x_1, \dots, x_n} \left\| \sum_{\substack{k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right\| \\ &\leq \sum_{x_1, \dots, x_n} \text{Tr} \left(\sum_{\substack{k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right) \\ &= \sum_{\substack{r=1 \\ r \neq i, j}}^n \sum_{x_r} \text{Tr} \left(\sum_{\substack{x_i, x_j \\ k=1 \\ k \neq i, j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right) \\ &= \sum_{\substack{r=1 \\ r \neq i, j}}^n \sum_{x_r} \text{Tr} \left(\sum_{b_1, \dots, b_n} G(b_1, \dots, b_n) \right) \end{aligned}$$

$$\begin{aligned}
&= \sum_{\substack{r=1 \\ r \neq i,j}}^n \sum_{x_r} \text{Tr}(\mathbb{1}_{d \times d}) \\
&= d \prod_{\substack{y=1 \\ y \neq i,j}}^n d_y.
\end{aligned} \tag{A17}$$

Hence, the first term in (A14) given by,

$$\sum_{x_1, \dots, x_n} \sum_{\substack{i,j \in \{1, \dots, n\} \\ i < j}} \left\| \sum_{\substack{k=1 \\ k \neq i,j}}^n \sum_{b_k} G(b_1, \dots, b_{i-1}, x_i, b_{i+1}, \dots, b_{j-1}, x_j, b_{j+1}, \dots, b_n) \right\| = d \sum_{\substack{i,j \in \{1, \dots, n\} \\ i < j}} \prod_{\substack{y=1 \\ y \neq i,j}}^n d_y \tag{A18}$$

By substituting the bounds from (A15)-(A18) in (A14), we obtain

$$S^C(n, \vec{d}, d) \leq \frac{1}{n \prod_y d_y} \left(d \sum_{\substack{i,j \in \{1, \dots, n\} \\ i < j}} \left(\prod_{\substack{y=1 \\ y \neq i,j}}^n d_y \right) + \prod_{y=1}^n d_y \right), \tag{A19}$$

which reduces to the first expression of (15).

For the other bound, let us use the fact that in (A5) only the term $G(x_1, x_2, \dots, x_n)$ occurs n times and all the other terms can occur at most $(n-1)$ times to get an upper bound on χ as follows

$$\chi \leq G(x_1, x_2, \dots, x_n) + (n-1) \sum_{b_1, \dots, b_n} G(b_1, \dots, b_n). \tag{A20}$$

Replacing this bound into (A4) and employing the triangle inequality for norm, we get

$$S^C(n, \vec{d}, d) \leq \frac{1}{n \prod_y d_y} \left(\sum_{x_1, \dots, x_n} \|G(x_1, \dots, x_n)\| + (n-1) \sum_{x_1, \dots, x_n} \left\| \sum_{b_1, \dots, b_n} G(b_1, \dots, b_n) \right\| \right). \tag{A21}$$

We already have a bound given by (A15) on the second sum in the above equation. The first term is bounded by d since

$$\begin{aligned}
\sum_{x_1, \dots, x_n} \|G(x_1, \dots, x_n)\| &\leq \sum_{x_1, \dots, x_n} \text{Tr}(G(x_1, \dots, x_n)) \\
&= \text{Tr} \left(\sum_{x_1, \dots, x_n} G(x_1, \dots, x_n) \right) \\
&= \text{Tr}(\mathbb{1}_{d \times d}) \\
&= d.
\end{aligned} \tag{A22}$$

Therefore, we arrive at

$$S^C(n, \vec{d}, d) \leq \frac{1}{n \prod_y d_y} \left(d + (n-1) \prod_y d_y \right), \tag{A23}$$

which reduces to the second expression of (15). This completes the proof. \square

Appendix B: Proof of Result 4

In order to provide a detailed proof of Result 4, we first state a general feature of communication tasks.

Lemma 1. Consider a general form of a linear function of $\{p(b_y|x, y)\}$,

$$S = \sum_{x, y, b_y} c_{x, y, b_y} p(b_y|x, y). \quad (\text{B1})$$

The maximum value of S within \mathcal{C}_d , which we denote by S^C , is obtained by deterministic strategies and can be written only in terms of decoding function $\{p_b(b_y|y, m)\}$.

Proof. Replacing the expression of $p(b_y|x, y)$ for classical communication (3) into (B1), we see that

$$\begin{aligned} S^C &= \max_{\substack{\{p_a(m|x, \lambda)\} \\ \{p_b(b_y|y, m, \lambda)\} \\ \{\pi(\lambda)\}}} \sum_x \left(\sum_{y, b_y} c_{x, y, b_y} p(b_y|x, y) \right) \\ &= \max_{\substack{\{p_a(m|x, \lambda)\} \\ \{p_b(b_y|y, m, \lambda)\} \\ \{\pi(\lambda)\}}} \int_{\lambda} \pi(\lambda) \left[\sum_x \left\{ \sum_m p_a(m|x, \lambda) \left(\sum_{y, b_y} c_{x, y, b_y} p_b(b_y|y, m, \lambda) \right) \right\} \right] d\lambda \\ &= \max_{\substack{\{p_b(b_y|y, m, \lambda)\} \\ \{\pi(\lambda)\}}} \int_{\lambda} \pi(\lambda) \left[\sum_x \max_m \left(\sum_{y, b_y} c_{x, y, b_y} p_b(b_y|y, m, \lambda) \right) \right] d\lambda. \end{aligned} \quad (\text{B2})$$

This is achieved when $p_a(m^*(\lambda)|x, \lambda) = 1$ for all x, λ , where for each λ , $m^*(\lambda)$ is defined as follows

$$\sum_{y, b_y} c_{x, y, b_y} p_b(b_y|y, m^*(\lambda), \lambda) \geq \sum_{y, b_y} c_{x, y, b_y} p_b(b_y|y, m, \lambda) \quad \forall m \in [d]. \quad (\text{B3})$$

Now, the above expression (B2) is a convex sum with respect to $\pi(\lambda)$ and thus, we can omit the dependence of λ by taking the best value of $[\sum_x \max_m (\sum_{y, b_y} c_{x, y, b_y} p_b(b_y|y, m, \lambda))]$ over different choices of λ as follows

$$S^C = \max_{\{p_b(b_y|y, m)\}} \left[\sum_x \max_m \left(\sum_{y, b_y} c_{x, y, b_y} p_b(b_y|y, m) \right) \right]. \quad (\text{B4})$$

Therefore, it is sufficient to consider deterministic decoding, that is, $p_b(b_y|y, m) \in \{0, 1\}$ to achieve S^C . Moreover, given any decoding strategy $\{p_b(b_y|y, m)\}$, the best encoding function is

$$p_a(m^*|x) = 1, \quad \text{where} \quad \sum_{y, b_y} c_{x, y, b_y} p_b(b_y|y, m^*) \geq \sum_{y, b_y} c_{x, y, b_y} p_b(b_y|y, m) \quad \forall m \in [d]. \quad (\text{B5})$$

This completes the proof. \square

Proof of Result 4. The proof is essentially a generalization of the proof given in Section II-A of [40], which was restricted for the particular case where $d = d_y$ for all y . We know from the above lemma that the optimal encoding and decoding functions are deterministic. Thus, this can be written in a functional form as

$$E(x_1 \cdots x_n) = m \quad \text{if} \quad p_a(m|x) = 1, \quad (\text{B6})$$

and

$$D_y(m) = b_y \quad \text{if} \quad p_b(b_y|y, m) = 1. \quad (\text{B7})$$

Here, $E(x_1 \cdots x_n)$ is a function whose domain is the set of inputs $x = x_1 \cdots x_n$ and range is the set messages $[d]$. And $D_y(m)$ is a function whose domain is the set of messages $[d]$ and range is the set $[d_y]$. We say the decoding strategy is ‘identity decoding’, denoted by $\{\tilde{D}_y\}$, if

$$\forall y, \tilde{D}_y(m) = m. \quad (\text{B8})$$

We want to show that, without loss of generality we can take $\{\tilde{D}_y\}$ for the maximum success probability. Consider an encoding $E(x)$ (B6) and a decoding $\{D_y\}$ (B7) that may not be $\{\tilde{D}_y\}$, that is, there may exists y such that $D_y(m) \neq m$. Let $D_y^{\leftarrow}(b_y)$ is the preimage of b_y , that is, $D_y^{\leftarrow}(b_y) = \{m \in [d] : D_y(m) = b_y\}$.

Subsequently, we consider the following quantity

$$D_1^{\leftarrow}(b_1) \cdots D_n^{\leftarrow}(b_n) = \{m_1 \cdots m_n : D_1(m_1) = b_1, \cdots, D_n(m_n) = b_n\}, \quad (\text{B9})$$

which is noting but the set of dit-string $\{m_1 \cdots m_n\}$ that is mapped to the sting $b_1 \cdots b_n$. We define another encoding function $\{\tilde{E}_x\}$ as follows

$$\tilde{E}(D_1^{\leftarrow}(x_1)D_2^{\leftarrow}(x_2) \cdots D_n^{\leftarrow}(x_n)) = m \text{ if } E(x_1 \cdots x_n) = m. \quad (\text{B10})$$

The above definition of \tilde{E} is not complete since it is not defined if $x_i \notin [d]$ since $D_y^{\leftarrow}(x_i) \in [d]$. In those cases, we take any encoding strategy. Now, we note that \tilde{E} is well-defined encoding function. Also note that \tilde{E} is a valid encoding for the random access codes considered by us only if $d \leq \min_y d_y$. Because, if $d > d_y$ for some y , then the domain of \tilde{E} may have a string of n dits that does not belong to x .

Suppose, for any input pair $x_1 \cdots x_n, y$ so that the encoding E and decoding $\{D_y\}$ guesses the correct dit x_y . Hence, if the encoding strategy is given by, $E(x = x_1 \cdots x_n) = m$, then the decoding strategy is given by, $D_y(m) = b_y = x_y$. Therefore, we have $D_y^{\leftarrow}(x_y) = m$. As a consequence, the new encoding \tilde{E}_x and the ‘identity decoding’ $\{\tilde{D}_y\}$ also provides the correct answer for at least one input pair from $\{D_1^{\leftarrow}(x_1)D_2^{\leftarrow}(x_2) \cdots D_n^{\leftarrow}(x_n)\}, y$. Hence, the average success probability for the strategy consisting of the encoding \tilde{E}_x and the ‘identity decoding’ $\{\tilde{D}_y\}$ is greater than or equal to that for the strategy with encoding E and decoding $\{D_y\}$. Therefore, we can consider ‘identity decoding’ without loss of generality.

Next, from Eq.(B4), the expression for S^C pertaining to the random access codes for ‘identity decoding’ can be written as

$$S^C = \frac{1}{n \prod_y d_y} \sum_x \max_m \left(\sum_y P(b_y = x_y | y, m) \right) = \frac{1}{n \prod_y d_y} \sum_x \max_m \left(\sum_y \delta_{x_y, m} \right), \quad (\text{B11})$$

and for the ‘identity decoding’, the best encoding can be determined from (B5) as follows

$$p_a(m^* | x) = 1, \text{ where } \sum_y \delta_{x_y, m^*} \geq \sum_y \delta_{x_y, m} \quad \forall m \in [d]. \quad (\text{B12})$$

Hence, the best encoding pertaining to the ‘identity decoding’ is just sending the dit that belongs to $[d]$ and occurs maximum times in the input string $x_1 \cdots x_n$.

Finally, we provide an expression for S^C for the best classical strategy derived above. In an input string $x_1 \cdots x_n$, say, the dit i occurs n_i number of times. The maximum value of a dit can be $\max_y d_y$. Alice sends message m such that $n_m = \max_{i=1, \dots, d} n_i$. As a result, out of n different values of y , they get success ($\max_{i=1, \dots, d} n_i$) times. As the total number of dits is n , the set of values of n_i should satisfy

$$\sum_{i=1}^{d_{\max}} n_i = n, \quad (\text{B13})$$

where $d_{\max} = \max_y d_y$. Moreover, dit i may not belongs to all $[d_y]$ and thus, n_i can not take all the solutions of the above equation. Say, k_i is the number of sets among $[d_1], \dots, [d_n]$ such that dit $i \in [d_y]$. Therefore, we are only interested in those solutions where $n_i \leq k_i$.

Given such a solution of $\{n_i\}$, there will be many possible number of input dit strings x having that $\{n_i\}$. Next, let us evaluate the number of input dit strings x that can have an arbitrary $\{n_i\}$. In any input string, at most $k_{d_{\max}}$ number of input dits can have the value d_{\max} . In the given set of input dit strings having $\{n_i\}$, the dit d_{\max} occurs $n_{d_{\max}}$ number of times. Hence, the dit d_{\max} can be arranged in $C_{n_{d_{\max}}}^{k_{d_{\max}}}$ different possible ways. Next, in any input string, at most $k_{d_{\max}-1}$ number of input dits can have the value $(d_{\max} - 1)$. However, among these $k_{d_{\max}-1}$ number of input dits, $n_{d_{\max}}$ number of dits have already taken the value d_{\max} in case of the given set of input strings. Also, in the given set of input dit strings having $\{n_i\}$, the dit $(d_{\max} - 1)$ occurs $n_{d_{\max}-1}$ number of times. Therefore, for any of the above-mentioned arrangements of the the dit d_{\max} , the dit $(d_{\max} - 1)$ can be arranged in $C_{n_{d_{\max}-1}}^{k_{d_{\max}-1} - n_{d_{\max}}}$ different possible ways. Proceeding in this way, it can be shown that an arbitrary dit j can be arranged in $C_{n_j}^{k_j}$ different possible

ways with $\alpha_j = k_j - \sum_{i=j+1}^{d_{\max}} n_i$ for any arrangement of the dits- $d_{\max}, (d_{\max} - 1), \dots, j + 1$. Therefore, given any $\{n_i\}$, there will be $\left(\prod_{j=1}^{d_{\max}} C_{n_j}^{\alpha_j}\right)$ (with $\alpha_j = k_j - \sum_{i=j+1}^{d_{\max}} n_i$) number of input dit strings having that $\{n_i\}$. Combining these facts we obtain (18). \square

Appendix C: Derivation of Eq.(21) and Eq.(22)

From Result 4, we can write the following for $n = 2, d_y = \tilde{d}$ for all y , and $d \leq \tilde{d}$,

$$S^C(2, \tilde{d}, d) = \frac{1}{2\tilde{d}^2} \sum_{\{n_i\} \in \mathcal{S}} \left[N_{\{n_i\}} \max_{i=1, \dots, \tilde{d}} \{n_i\} \right] \quad (\text{C1})$$

where $N_{\{n_i\}}$ is the number of input dit strings having a given $\{n_i\}$; and \mathcal{S} denotes the set of $\{n_i\}$ satisfying

$$\sum_{i=1}^{\tilde{d}} n_i = 2 \quad (\text{C2})$$

such that $n_i \leq 2$ for all i .

Next, let us characterize the set \mathcal{S} . It can be noted that there are the following two types of $\{n_i\} \in \mathcal{S}$:

1. For each $i \in [\tilde{d}]$, $n_i = 2$ and $n_j = 0$ for all $j \neq i$ and $j \in [\tilde{d}]$.

There are \tilde{d} number of such $\{n_i\} \in \mathcal{S}$. However, $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 0$ for each of those $\{n_i\} \in \mathcal{S}$ satisfying $n_i = 2$ for any i such that $i \in \{d+1, \dots, \tilde{d}\}$ and $n_j = 0$ for all $j \in [\tilde{d}]$ and $j \neq i$. Hence, only d number of $\{n_i\} \in \mathcal{S}$ belonging to this class contribute to the sum of (C1). It is straightforward to check that for each of these d number of $\{n_i\} \in \mathcal{S}$, $N_{\{n_i\}} = 1$ and $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 2$.

2. For each $i, j \in [\tilde{d}]$ with $i \neq j$, $n_i = n_j = 1$ and $n_k = 0$ for all $k \notin \{i, j\}$ with $k \in [\tilde{d}]$.

There are $C_2^{\tilde{d}}$ number of such $\{n_i\} \in \mathcal{S}$. However, $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 0$ for each of those $\{n_i\} \in \mathcal{S}$ satisfying $n_i = n_j = 1$ for any i, j with $i \neq j, i, j \in \{d+1, \dots, \tilde{d}\}$ and $n_k = 0$ for all $k \in [\tilde{d}], k \neq i, k \neq j$. There are $C_2^{(\tilde{d}-d)}$ number of such $\{n_i\} \in \mathcal{S}$ satisfying this. Hence, only $C_2^{\tilde{d}} - C_2^{(\tilde{d}-d)}$ number of $\{n_i\} \in \mathcal{S}$ belonging to this second class contribute to the sum of (C1). It can be checked that for each of these $C_2^{\tilde{d}} - C_2^{(\tilde{d}-d)}$ number of $\{n_i\} \in \mathcal{S}$, $N_{\{n_i\}} = 2$ and $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 1$.

Therefore, we have from Eq.(C1)

$$\begin{aligned} S^C(2, \tilde{d}, d) &= \frac{1}{2\tilde{d}^2} \left[2d + 2 \left(C_2^{\tilde{d}} - C_2^{(\tilde{d}-d)} \right) \right] \\ &= \frac{1}{2\tilde{d}^2} \left[d + 2d\tilde{d} - d^2 \right]. \end{aligned} \quad (\text{C3})$$

Similarly, following the same analysis as above, we can get the expression for $n = 3, d_y = \tilde{d}$ for all y , and $d \leq \tilde{d}$,

$$S^C(3, \tilde{d}, d) = \frac{1}{3\tilde{d}^3} \sum_{\{n_i\} \in \mathcal{S}} \left[N_{\{n_i\}} \max_{i=1, \dots, \tilde{d}} \{n_i\} \right] \quad (\text{C4})$$

where $N_{\{n_i\}}$ is the number of input dit strings with a given $\{n_i\}$; and \mathcal{S} denotes the set of $\{n_i\}$ satisfying

$$\sum_{i=1}^{\tilde{d}} n_i = 3 \quad (\text{C5})$$

such that $n_i \leq 3$ for all i . Now there are three cases that satisfy Eq.(C5):

1. For each $i \in [\tilde{d}]$, $n_i = 3$ and $n_j = 0$ for all $j \neq i$ and $j \in [\tilde{d}]$.

There are \tilde{d} number of such $\{n_i\} \in \mathcal{S}$. However, $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 0$ for each of those $\{n_i\} \in \mathcal{S}$ satisfying $n_i = 3$ for any i with $i \in \{d+1, \dots, \tilde{d}\}$ and $n_j = 0$ for all $j \in [\tilde{d}]$ and $j \neq i$. Hence, only d number of $\{n_i\} \in \mathcal{S}$ belonging to this class contribute to the sum of (C4). For each of these d number of $\{n_i\} \in \mathcal{S}$, we have that $N_{\{n_i\}} = 1$ and $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 3$. Hence, the contribution to the sum is $3d$.

2. For each $i, j, k \in [\tilde{d}]$ with $i \notin \{j, k\}$, $j \notin \{i, k\}$, $k \notin \{i, j\}$, $n_i = n_j = n_k = 1$ and $n_l = 0$ for all $l \notin \{i, j, k\}$ and $l \in [\tilde{d}]$.

There are $C_3^{\tilde{d}}$ number of such $\{n_i\} \in \mathcal{S}$. Moreover, $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 0$ for each of those $\{n_i\} \in \mathcal{S}$ satisfying $n_i = n_j = n_k = 1$ for any choice of i, j, k with $i, j, k \in \{d+1, \dots, \tilde{d}\}$, $i \notin \{j, k\}$, $j \notin \{i, k\}$, $k \notin \{i, j\}$ and $n_l = 0$ for all $l \in [\tilde{d}]$ and $l \notin \{i, j, k\}$. There are $C_3^{(\tilde{d}-d)}$ number of such $\{n_i\} \in \mathcal{S}$ satisfying this. Thus, only $C_3^{\tilde{d}} - C_3^{(\tilde{d}-d)}$ number of $\{n_i\} \in \mathcal{S}$ belonging to this class contribute to the sum of (C4). It can be checked that for each of these $C_3^{\tilde{d}} - C_3^{(\tilde{d}-d)}$ number of $\{n_i\} \in \mathcal{S}$, $N_{\{n_i\}} = 3!$ and $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 1$. Therefore, the contribution to the sum will be $(3!) \left(C_3^{\tilde{d}} - C_3^{(\tilde{d}-d)} \right)$.

3. For each $i, j \in [\tilde{d}]$ with $i \neq j$, $n_i = 2$, $n_j = 1$ and $n_k = 0$ for all $k \notin \{i, j\}$ with $k \in [\tilde{d}]$.

The feasible solutions of Eq.(C5) that contribute to the Eq.(C4) are of two types:

(A) $i \in [d]$ and $j \in [\tilde{d}] - \{i\}$. The number of possible such $\{n_i\} \in \mathcal{S}$ is given by, $d(\tilde{d} - 1)$. Also, for each such $\{n_i\}$, we have that $N_{\{n_i\}} = 3$ and $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 2$. Therefore, the contribution to the sum appearing in Eq.(C4) by this case is $6d(\tilde{d} - 1)$.

(B) $i \in \{d+1, \dots, \tilde{d}\}$ and $j \in [d]$. The number of possible such $\{n_i\} \in \mathcal{S}$ is given by, $d(\tilde{d} - d)$. And for each such $\{n_i\}$, we have that $N_{\{n_i\}} = 3$ and $\max_{i=1, \dots, \tilde{d}} \{n_i\} = 1$. Hence, the contribution to the sum appearing in Eq.(C4) for this case is given by, $3d(\tilde{d} - d)$.

Therefore, the total contribution to the sum of Eq.(C4) is given by, $6d(\tilde{d} - 1) + 3d(\tilde{d} - d) = 3d(3\tilde{d} - d - 2)$.

Therefore, we have from Eq. (22) that

$$\begin{aligned} S^C(3, \tilde{d}, d) &= \frac{1}{3\tilde{d}^3} \left[(3!) \left(C_3^{\tilde{d}} - C_3^{\tilde{d}-d} \right) + 3d(3\tilde{d} - d - 2) + 3d \right] \\ &= \frac{d}{3\tilde{d}^3} \left(d^2 - 1 + 3\tilde{d}(\tilde{d} + 1 - d) \right). \end{aligned} \quad (\text{C6})$$

Appendix D: Proof of Result 5

Let us take three arbitrary orthonormal basis $\{|\psi_1^1\rangle, |\psi_2^1\rangle\}$, $\{|\psi_1^2\rangle, |\psi_2^2\rangle\}$, $\{|\psi_1^3\rangle, |\psi_2^3\rangle\}$ in \mathbb{C}^2 such that $M_{x_y|y} = |\psi_{x_y}^y\rangle\langle\psi_{x_y}^y|$ with $x_y \in [2]$ for all $y \in \{1, 2, 3\}$. A unitary can always be applied to these three measurements. Therefore, without any loss of generality, we can assume that

$$|\psi_{x_1}^1\rangle\langle\psi_{x_1}^1| = \frac{1}{2} [\mathbb{1} + (-1)^{x_1}\sigma_z] \quad \text{with } x_1 \in [2], \quad (\text{D1})$$

$$|\psi_{x_2}^2\rangle\langle\psi_{x_2}^2| = \frac{1}{2} \left[\mathbb{1} + (-1)^{x_2} \left(\alpha\sigma_z + \sqrt{1-\alpha^2}\sigma_x \right) \right] \quad \text{with } x_2 \in [2], \quad (\text{D2})$$

$$|\psi_{x_3}^3\rangle\langle\psi_{x_3}^3| = \frac{1}{2} \left[\mathbb{1} + (-1)^{x_3} \left(\beta\sigma_z + \gamma\sqrt{1-\beta^2}\sigma_x \pm \sqrt{1-\beta^2}\sqrt{1-\gamma^2}\sigma_y \right) \right] \quad \text{with } x_3 \in [2]. \quad (\text{D3})$$

where $-1 \leq \alpha, \beta, \gamma \leq 1$.

For the above-mentioned given set of three rank-one projective qubit measurements, the maximum average success probability in quantum theory is given by,

$$S^C(n=3, \tilde{d}=2, d=2) = \frac{1}{24} \sum_{x_1, x_2, x_3=1}^2 \|M_{x_1|1} + M_{x_2|2} + M_{x_3|3}\|. \quad (\text{D4})$$

By definition, $\|M_{x_1|1} + M_{x_2|2} + M_{x_3|3}\|$ is nothing but the maximum eigenvalue of $(M_{x_1|1} + M_{x_2|2} + M_{x_3|3})$, which can be evaluated easily. Subsequently, it can be checked that

$$\begin{aligned} \sum_{x_1, x_2, x_3=1}^2 \|M_{x_1|1} + M_{x_2|2} + M_{x_3|3}\| &= 12 + \sqrt{3 + 2\alpha - 2\beta - 2\alpha\beta - 2\gamma\sqrt{1 - \alpha^2}\sqrt{1 - \beta^2}} \\ &\quad + \sqrt{3 - 2\alpha + 2\beta - 2\alpha\beta - 2\gamma\sqrt{1 - \alpha^2}\sqrt{1 - \beta^2}} \\ &\quad + \sqrt{3 - 2\alpha - 2\beta + 2\alpha\beta + 2\gamma\sqrt{1 - \alpha^2}\sqrt{1 - \beta^2}} \\ &\quad + \sqrt{3 + 2\alpha + 2\beta + 2\alpha\beta + 2\gamma\sqrt{1 - \alpha^2}\sqrt{1 - \beta^2}}. \end{aligned} \quad (\text{D5})$$

We have found out the minimum of the above expression (D5) by performing numerical optimization. It turns out that

$$\min_{\alpha, \beta, \gamma \in [-1, 1]} \left(\sum_{x_1, x_2, x_3=1}^2 \|M_{x_1|1} + M_{x_2|2} + M_{x_3|3}\| \right) = 18. \quad (\text{D6})$$

In other words,

$$\min_{\alpha, \beta, \gamma \in [-1, 1]} (\xi_1 + \xi_2 + \xi_3 + \xi_4) = 6, \quad (\text{D7})$$

where

$$\begin{aligned} \xi_1 &= \sqrt{3 + 2\alpha - 2\beta - 2\alpha\beta - 2\gamma\sqrt{1 - \alpha^2}\sqrt{1 - \beta^2}}, \\ \xi_2 &= \sqrt{3 - 2\alpha + 2\beta - 2\alpha\beta - 2\gamma\sqrt{1 - \alpha^2}\sqrt{1 - \beta^2}}, \\ \xi_3 &= \sqrt{3 - 2\alpha - 2\beta + 2\alpha\beta + 2\gamma\sqrt{1 - \alpha^2}\sqrt{1 - \beta^2}}, \\ \xi_4 &= \sqrt{3 + 2\alpha + 2\beta + 2\alpha\beta + 2\gamma\sqrt{1 - \alpha^2}\sqrt{1 - \beta^2}}. \end{aligned}$$

In order to prove Result 5, it is sufficient to show that $(\xi_1 + \xi_2 + \xi_3 + \xi_4) = 6$ only if the three projective measurements are compatible, or $(\alpha, \beta, \gamma) = \{(\pm 1/2, \pm 1/2, -1), (\pm 1/2, \mp 1/2, 1)\}$.

Since $-1 \leq \alpha, \beta, \gamma \leq 1$, we divide the regions of α, β and γ into the following sub-regions:

- i. $\alpha, \beta, \gamma \in [0, 1]$,
- ii. $\alpha \in [-1, 0]; \beta, \gamma \in [0, 1]$,
- iii. $\alpha, \beta \in [-1, 0]; \gamma \in [0, 1]$,
- iv. $\alpha, \beta, \gamma \in [-1, 0]$,
- v. $\alpha, \gamma \in [0, 1]; \beta \in [-1, 0]$,
- vi. $\alpha, \gamma \in [-1, 0]; \beta \in [0, 1]$,
- vii. $\alpha, \beta \in [0, 1]; \gamma \in [-1, 0]$,
- viii. $\alpha \in [0, 1]; \beta, \gamma \in [-1, 0]$.

We start by considering the above-mentioned sub-region (i), i.e., $\alpha, \beta, \gamma \in [0, 1]$. In this case, we note the following holds from numerical evaluation,

$$\min_{\alpha, \beta, \gamma \in [0, 1]} (\xi_1 + \xi_2) = 2, \quad (\text{D8})$$

and

$$\min_{\alpha, \beta, \gamma \in [0,1]} (\zeta_3) \geq \min_{\alpha, \beta \in [0,1]} \sqrt{3 - 2\alpha - 2\beta + 2\alpha\beta} = 1, \quad (\text{D9})$$

since the derivative of the above expression is zero at $\alpha = 1$ or/and $\beta = 1$.

Next, we evaluate the maximum as well as minimum of $(\zeta_1 + \zeta_2 + \zeta_3)$ numerically under the constraint that $(\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4) = 6$. It is obtained that

$$\min_{\alpha, \beta, \gamma \in [0,1]} (\zeta_1 + \zeta_2 + \zeta_3) = \max_{\alpha, \beta, \gamma \in [0,1]} (\zeta_1 + \zeta_2 + \zeta_3) = 3, \quad \text{when } \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6. \quad (\text{D10})$$

Therefore, we have that

$$\zeta_1 + \zeta_2 + \zeta_3 = 3, \quad \text{when } \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6. \quad (\text{D11})$$

Hence, the following is implied from (D8), (D9), (D11),

$$\zeta_1 + \zeta_2 = 2, \quad \zeta_3 = 1, \quad \text{and } \zeta_4 = 3, \quad \text{when } \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6. \quad (\text{D12})$$

Next, it can be checked that $\zeta_3 = 1$ only if $\alpha = 1$ or/and $\beta = 1$. Now, when $\alpha = 1$, then $\zeta_4 = 3$ implies that $\beta = 1$. Similarly, when $\beta = 1$, then $\zeta_4 = 3$ implies that $\alpha = 1$. Therefore, when $\alpha, \beta, \gamma \in [0, 1]$, then $(\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4) = 6$ holds only if $\alpha = \beta = 1$.

Next, consider the sub-region (iii), i.e., for $\alpha, \beta \in [-1, 0]$; $\gamma \in [0, 1]$. We note that if $\alpha \rightarrow -\alpha$ and $\beta \rightarrow -\beta$ then the four expressions ζ_i interchange among themselves as we can readily verify $\zeta_1 \rightarrow \zeta_2$, $\zeta_2 \rightarrow \zeta_1$, $\zeta_3 \rightarrow \zeta_4$, $\zeta_4 \rightarrow \zeta_3$. Thus, following the similar calculation for the sub-region (i), we find that $\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6$ holds only if $\alpha = \beta = -1$. Similarly, for sub-regions (vi) and (viii), one can show that $\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6$ holds only if $-\alpha = \beta = 1$ and $\alpha = -\beta = 1$, respectively.

Next, let us focus on the sub-region (iv), i.e., when $\alpha, \beta, \gamma \in [-1, 0]$. In this case, we obtain the following by performing numerical optimizations,

$$\begin{aligned} \min_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_1 + \zeta_4) &= \max_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_1 + \zeta_4) = 2, \quad \text{when } \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6, \\ \min_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_2 + \zeta_4) &= \max_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_2 + \zeta_4) = 2, \quad \text{when } \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6, \\ \min_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_1 + \zeta_3) &= \max_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_1 + \zeta_3) = 4, \quad \text{when } \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6, \\ \min_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_2 + \zeta_3) &= \max_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_2 + \zeta_3) = 4, \quad \text{when } \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6. \end{aligned}$$

Hence, we can infer that whenever $\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6$,

$$\zeta_1 + \zeta_4 = \zeta_2 + \zeta_4 = 2, \quad \zeta_1 + \zeta_3 = \zeta_2 + \zeta_3 = 4. \quad (\text{D13})$$

Therefore, we have $\zeta_1 = \zeta_2$ if $\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 6$. Also, it can be easily checked from the expressions of $\zeta_1, \zeta_2, \zeta_3$ and ζ_4 that

$$\zeta_1^2 + \zeta_2^2 + \zeta_3^2 + \zeta_4^2 = 12. \quad (\text{D14})$$

By putting $\zeta_1 = \zeta_2 = \zeta$, $\zeta_3 = 4 - \zeta$, $\zeta_4 = 2 - \zeta$, we get from (D14) that

$$2\zeta^2 + (4 - \zeta)^2 + (2 - \zeta)^2 = 12. \quad (\text{D15})$$

The possible solutions of the above equation are $\zeta = 1$ and $\zeta = 2$.

Before proceeding, let us point out the following observations that can be checked numerically,

$$\min_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_1) = \min_{\alpha, \beta, \gamma \in [-1, 0]} (\zeta_2) = 1. \quad (\text{D16})$$

First we take $\zeta = 1$. It can be shown that $\alpha, \beta, \gamma \in [-1, 0]$, $\zeta_1 = \zeta_2 = 1$ only if $\alpha = -1$ and $\beta = -1$. Next, let us take $\zeta = 2$. Consequently, we have that $\zeta_1 = \zeta_2 = 2$, $\zeta_3 = 2$, $\zeta_4 = 0$. It can be checked that the unique solution of these

four equations is given by, $\alpha = -1/2, \beta = -1/2, \gamma = -1$.

Next, we remark that for the remaining sub-regions (ii),(v),(vii) wherein the variables α, β, γ changes their signs with respect to the sub-region (iv) where $\alpha, \beta, \gamma \in [-1, 0]$, the four expressions ξ_i interchange among themselves. Thus, a similar calculation applies to these three regions and consequently, the solution for $\xi_1 + \xi_2 + \xi_3 + \xi_4 = 6$ are the same with the appropriate signs.

Finally, let us note that there are, in general, two cases where we do not observe any advantage. Firstly, $\alpha = \pm 1$ and $\beta = \pm 1$, which implies that the three measurements $\{M_{x_1|1}\}, \{M_{x_2|2}\}$ and $\{M_{x_3|3}\}$ are compatible. Secondly, $(\alpha, \beta, \gamma) = \{(\pm 1/2, \pm 1/2, -1), (\pm 1/2, \mp 1/2, 1)\}$, which are obtained in sub-regions (iv),(ii),(v),(vii), implies that the three measurements are incompatible. This completes the proof.