Certifying the purity of quantum states with temporal correlations

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Correlations obtained from sequences of measurements have been employed to distinguish among different physical theories or to witness the dimension of a system. In this work we show that they can also be used to establish semi-device independent lower bounds on the purity of the initial quantum state or even on one of the post-measurement states. For single systems this provides information on the quality of the preparation procedures of pure states or the implementation of measurements with anticipated pure post-measurement states. For joint systems one can combine our bound with results from entanglement theory to infer an upper bound on the concurrence based on the temporal correlations observed on a subsystem.

I. INTRODUCTION

Many applications in quantum information theory such as teleportation [1] and measurement-based quantum computation [2] use as a resource pure entangled states. That is, ideally the corresponding protocols are applied to the respective pure resource state and deviations from this resource may result in errors [1][3] and lead to the need of entanglement purification [4][5] or fault tolerant implementations (see e.g. [6][5]) if one takes into account also imperfections after the preparation procedure. Due to interactions with the environment in experiments often mixed states are prepared instead of the desired pure state. By knowing how much the prepared state differs from a pure state one obtains some intuition on the quality of the preparation process without attaining to full tomography. However, it should be noted that the purity only provides information about how much the prepared state deviates from a pure one (which might not necessarily be the desired one).

The purity of a quantum state can be quantified via

$$\mathcal{P}(\varrho) = \text{tr}[(\varrho)^2].$$

The purity attains its maximal value of 1 for pure states and its minimal value of 1/d for the maximally mixed state for d-dimensional systems. It is related to the linear entropy $S_L(\varrho) = 1 - \mathcal{P}(\varrho)$ and the Renyi-2 entropy $\mathcal{P}_2(\varrho) = \log_2(d \mathcal{P}(\varrho))$. The purity of quantum states has been also studied from a resource-theoretic point of view [10]. Moreover, the task of distilling local pure states via a subclass of local operations and classical communication has been considered [11].

It is well known that the purity (of subsystems) of bipartite systems and their entanglement are connected. States for which the purity of the whole system is sufficiently small have to be separable, as there exists a set containing only separable states around the maximally mixed state which has a finite volume [13][14]. For two-qubit pure states any entanglement measure can be written as a function of the purity of one of its subsystems as in this case the purity uniquely determines the set of Schmidt coefficients and any entanglement measure for bipartite pure states is a function of the Schmidt coefficients [15]. For mixed (or higher-dimensional) states the relation among entanglement and sub-system purity is no one-to-one correspondence anymore, however, for example lower [10] and upper [17] bounds based on the purity of a subsystem and total system have been shown for the concurrence $C(\varrho)$ [19][20], which is an entanglement measure. In particular, it has been shown that

$$\max_{X \in \{A,B\}} 2\{\text{tr}[(\varrho)^2] - \text{tr}[(g_X)^2]\} \leq |C(\varrho)|^2$$

and

$$|C(\varrho)|^2 \leq \min_{X \in \{A,B\}} 2\{1 - \text{tr}[(g_X)^2]\},$$

where $g_X$ is the reduced state of subsystem $X$. The first bound captures quantitatively the observation that only for entangled states the reduced states can be more mixed than the state of the whole system [18]. The upper and lower bound in the equation above can be determined in an experiment by measuring local observables using two identical copies of the state $\varrho$ [16][17]. The purity (or Renyi-n entropies) of a system can also be experimentally measured by employing two copies of the state (see e.g. [21][25] and references therein) or by performing randomized measurements [26][29].

By performing tomography on the system one could reconstruct the state and calculate the purity of the system exactly. In particular, there exist adaptive schemes [30][31] for which fewer measurement settings have to be implemented. However, it should be noted that as in any tomographic approach the measurements are required to be characterized (at least to some extend). The relation of the scaling of the accuracy in device-dependent adaptive process tomography and the purity of the measured state has been studied [32].

Device-independent bounds on the linear entropy (of the total system) or the concurrence can be also obtained from the value of violation of a Bell inequality [33][34]. Moreover, device-independent entropy witnesses based on dimension witnesses have been proposed in the context of prepare-and-measure scenarios [35] and sector lengths which are related to the average purity of reduced states have been studied (see e.g. [36][38] and references therein)
Here we propose to use the temporal correlations obtained from sequences of measurements on a single copy to deduce a semi-device-independent lower bound on the purity. This approach relies only on the assumption of the dimension of the measured (sub)system and that measurements can be repeated (see below for more details). Note that even though for a single qubit system less measurements are required in a tomographic approach than in our approach such schemes require knowledge about the measurements that are implemented. Moreover, our approach does not require to prepare two identical copies of the state at the same time and to act non-locally on the subsystems of different copies [44]. It is straightforward to see from the equations above that a lower bound on the purity of a (sub)system provides an upper bound on the linear entropy or the concurrence.

Our approach uses sequential measurements and is conceptually different from the ones previously studied. In particular, we can also give a lower bound on the maximal purity of the post-measurement state at the second time step for outcome ”+” provided the purity of the initial state is known.

The paper is organized as follows. First we will describe the sequential scenario we are interested in and explain how one can obtain lower bounds on the purity of the initial or one of the post-measurement states from the observed temporal correlations. Then we will discuss some known results on the relation among entanglement and the purity of the reduced states for bipartite systems which can be used to obtain an upper bound on the concurrence. Finally we will provide a summary and an outlook.

Using temporal correlations to obtain a lower bound on the purity. — We will consider in the following sequences of general measurements acting on a single (sub)system whose (reduced) state is $\varrho_m$ (see Fig. 1). To be more precise, we will examine the correlations $p(ab|xy)$ which correspond to the probability for obtaining outcome ”$a$” in a first time step if one performs measurement ”$x$” and then observing outcome ”$b$” in a second time step if measurement ”$y$” is performed.

We will assume that one can use the same measurement apparatus at different time steps and the labeling of measurement settings does not change, i.e. in case $x=y$ one performs the same measurement twice, however, the outcomes do not need to be the same. The only further assumption will be that in the following the (sub)system that is measured is a two-dimensional system. In particular, we will not restrict the type of measurements, i.e. arbitrary instruments are allowed.

We consider the following quantity:

$$B_1 = p(+|00) + p(+|11) + p(-|01) + p(-|10).$$

This scenario and the quantity $B_1$ have been studied in [42] and it has been shown there that one can provide an (non-trivial) upper bound for general measurements on a qubit which allows to employ $B_1$ also as a dimension witness.
and then prepares the state $\frac{1}{2}(1 - \vec{\alpha}_i \cdot \vec{\sigma})$. The other measurement measures the observable $\vec{\alpha}_i \cdot \vec{\sigma}$.

If one obtains in an experiment a value for $B_1$ denoted here and in the following by $B_1^{exp}$ one can straightforwardly deduce a lower bound on the purity of the measured initial state. This is due to the fact that $B_1(p)$ is a monotonically increasing function of $P$ [see Eq. (5)] and $B_1(p) \geq B_1^{exp}$ if the purity of the initial state that is measured in the experiment is given by $P = 1/2(1 + p^2)$. The last relation captures that in an experiment the measurements that are implemented do not need to be the optimal ones that allow one to attain $B_1(p)$. With this one obtains that in order to observe $B_1^{exp}$ a certain amount of purity is required. In particular, we obtain the following observation.

**Observation 1.** Let $B_1^{exp}$ be the value for $B_1$ obtained in an experiment by performing sequences of measurements on the state $\varrho_i$. Then it holds for the purity $P$ of $\varrho_i$ that

$$P \geq \frac{(2B_1^{exp} - 5)^2 + 1}{2}. \quad (6)$$

Hence, temporal correlations allow one to witness the initial purity.

Knowing the purity of the initial state it is also possible to deduce a lower bound on the maximal purity of the post-measurement state occurring at the second time step for outcome “+”. To be more precise, one can provide a lower bound on the state measured in the second time step, which here and in the following we will refer to as post-measurement state. Let $p$ be the length of the Bloch vector of the initial state $\varrho_i$ and $w_{+|i}$ the one of the post-measurement state that is obtained after performing measurement $i \in \{0, 1\}$ on $\varrho_i$ and observing outcome “+”. Then one can determine the maximum $B_1(p, w_{+|0}, w_{+|1})$ that is attainable with all measurements and states that respect the imposed purities. One can show that $B_1(p, w_{+|0}, w_{+|1})$ is monotonically increasing as a function of $W = 1/2(1 + w^2)$ (assuming the other purities fixed but arbitrary). Moreover, in an experiment leading to $B_1^{exp}$ in which the states occur with the respective purities it might be that one deviates from the optimal protocol. Hence, it holds for $w_{\text{max}} = \max_{i \in \{0, 1\}} w_{+|i}$ that

$$B_1(p, w_{\text{max}}, w_{\text{max}}) \geq B_1(p, w_{+|0}, w_{+|1}) \geq B_1^{exp}.$$ 

It only remains to determine $B_1(p, w) = B_1(p, w, w)$ to provide an explicit lower bound on the maximal purity of the post-measurement states of outcome ”+” depending on the purity of the input state. In the following theorem we provide a closed formula for $B_1(p, w)$ (see also Fig. 3).

**Theorem 2.** Let $P$ be the purity of the initial state and $W$ the purity of the post-measurement states that occur for measurement $i \in \{0, 1\}$ observing outcome ”+”. Then for a two-dimensional system the maximal value of $B_1$, $B_1(p, w)$, that can be obtained for arbitrary initial states and measurements that respect these constraints on the purities, is given by

$$B_1(p, w) = \begin{cases} \frac{2}{1 + \frac{1+w}{2} + \frac{(1+p)(1+w)}{4}} & 0 \leq w \leq \frac{1-p}{3+p} \\ \frac{1-p}{3+p} & \frac{1-p}{3+p} < w \leq 1 \end{cases}$$

where $w = \sqrt{2W - 1}$ and $p = \sqrt{2P - 1}$ are the length of the Bloch vector for the respective purity.

The proof of this theorem can be found in Appendix [B].

This theorem allows one to deduce a lower bound on the maximal purity of the post-measurement states provided that the purity of the initial state is known. In particular,
we have that for $\mathcal{B}_{1\text{exp}}^{\text{exp}} \leq 2$ we cannot deduce a lower bound, however if $\mathcal{B}_{1\text{exp}}^{\text{exp}} > 2$ it follows from the Theorem above and $B_1(p, w_{\text{max}}) \geq \mathcal{B}_{1\text{exp}}^{\text{exp}}$ that

$$W_{\text{max}} \geq \frac{14 + 4(\mathcal{B}_{1\text{exp}}^{\text{exp}})^2 + P + 5\sqrt{2P - 1}}{4 + P + 3\sqrt{2P - 1}} - \frac{2\mathcal{B}_{1\text{exp}}^{\text{exp}}(7 + \sqrt{2P - 1})}{4 + P + 3\sqrt{2P - 1}}. \quad (7)$$

Moreover, note that as $B_1(p, w)$ is monotonically increasing as a function of $\mathcal{W}$ we also have that

$$B_1(p) = \max_{0 \leq w \leq 1} B_1(p, w) = B_1(p, 1) = B_1(p) = \frac{5 + p}{2}, \quad (8)$$

which allows to bound the purity of the initial state as argued above [see Eq. (5)] and Observation 1.

**Upper bound on the concurrence based on the purity.**—
As mentioned before it is well known that for bipartite pure states there is a close connection between entanglement and the purity of the reduced state of a single party. In particular, the reduced state is pure only for product states, whereas for maximally entangled states it is maximally mixed. For mixed states and on a more quantitative level, entanglement measures such as the concurrence are defined as the convex roof extension of a function of the local purity. More precisely, the concurrence [19, 20] is given by

$$C(\rho) = \inf \sum_i q_i C(|\psi_i\rangle), \quad (9)$$

where the infimum is taken over all pure state decompositions, $\rho = \sum_i q_i |\psi_i\rangle \langle \psi_i|$, and $C(|\psi_i\rangle) = \sqrt{2[1 - \text{tr}(|\rho_A|^2)]}$ with $\rho_A = \text{tr}_B(|\psi_i\rangle \langle \psi_i|)$. It seems therefore natural to consider the relation among the concurrence and the purity of the reduced state more closely in order to obtain a bound on the concurrence. The following result will allow us to provide a upper bound on the concurrence based on the observed temporal correlations. For two-qubit states $\rho_{AB}$ with $\rho_A = \text{tr}_B(\rho_{AB})$ and $\rho_B = \text{tr}_A(\rho_{AB})$ it holds that [17]

$$C(\rho) \leq \min_{X \in \{A, B\}} \sqrt{2[1 - \text{tr}(|\rho_X|^2)]}. \quad (10)$$

This bound has been already observed for arbitrary bipartite $d$-dimensional states in [17]. For completeness we will nevertheless present in Appendix C a (alternative but similar) proof for two-qubit states. Combining this with the lower bound on the purity based on temporal correlations (see Observation 1) we can state the following observation.

**Observation 3.** Let $\rho_{AB}$ be a two-qubit state and $\mathcal{B}_{1\text{exp}}^{\text{exp}}$ the experimental value for $B_1$ obtained for sequences of measurements on one of the subsystems. Then it holds for the concurrence $C(\rho_{AB})$ that

$$C(\rho_{AB}) \leq \sqrt{1 - (2\mathcal{B}_{1\text{exp}}^{\text{exp}} - 5)^2}. \quad (11)$$

Moreover, it has been also shown in [17] that for multipartite states $C(\rho) \leq 2^{1 - n/2}\sqrt{2^n - 2 - \sum_i \text{tr}(|\varphi_i|^2)}$. Here $C(\rho)$ is a generalization of the concurrence to the multipartite case defined by $C(\psi) = 2^{1 - n/2}\sqrt{2^n - 2 - \sum_i \text{tr}(|\varphi_i|^2)}$ [10] [11], where $n$ is the number of parties, $\varphi_i$ are the single-party density matrices, and $C(\rho)$ is obtained via the convex roof extension from $C(\psi)$ (see Eq. (9)).

Hence, also for multipartite systems one can first obtain from the correlations that arise from sequences of local measurements on subsystems a semi-device-independent lower bound on the purity of the subsystems and with this then an upper bound on the concurrence of the joint system.

**Summary and outlook.**— In this work we considered sequential measurements on a qubit. We showed that one can deduce from the observed correlations a lower bound on the purity of the initial state of the qubit. In case the qubit is part of a two-qubit system, this provides an upper bound on the concurrence. Moreover, provided that the purity of the initial state is known our approach allows one to obtain a lower bound on the maximal purity of the post-measurement states occurring at the second time step for one of the outcomes. Our result shows that it is possible to use temporal correlations for bounds on the purity and the concurrence by considering explicitly the example of a qubit. Moreover, we proved that also for higher-dimensional systems it is essentially possible to employ temporal correlations in order to establish bounds on the purity. It would be relevant to pursue our investigation of higher-dimensional systems and provide explicit purity witnesses. Moreover, it would be interesting to see whether longer sequences allow in principle for a better performance as has been observed for the case of dimension witnesses [43].

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**Appendix A: Temporal correlations allow to witness the purity for $d$-dimensional systems**

In this Appendix we show that it is essentially possible to use temporal correlations for providing lower bounds on the purity for $d$-dimensional systems. In particular, we will prove that one can construct functions of the correlations whose maximum for arbitrary measurements is
(strictly) monotonically increasing as a function of the purity of the initial state. Hence, in order to observe a certain value of this function one has to have a certain amount of purity and therefore these can be used to provide lower bound on the purity. Moreover, we will show that in principle the quantity $B_1$ could also be used to witness the purity for $d$-dimensional systems.

**Proof.** In order to do so, we consider a quantity $R = \sum \alpha_{abxy} p(ab|xy)$, which is linear in the correlations and therefore also in the initial state. More precisely, it holds that $p(ab|xy) = p(a|x)p(b|xy) = tr(\hat{E}_{a|x} \hat{g}_m)tr(\hat{b}(a|xy))$ with $\hat{E}_{a|x}$ being the effect for the measurement in the first time step. Now let us assume that for a given purity of the initial state $P$ one knows the optimal protocol that maximize $R$. We then have $P = \sum q_i^2$ with $q_i$ being the eigenvalues of the optimal $\hat{g}_m$. Let us denote the eigenbasis for $\hat{g}_m$ by $\{|i\rangle\}$, the corresponding optimal effects by $\hat{E}_{a|x}$ and the maximal attainable value by $R(P)$. Then one obtains that

$$R(P) = \sum_{i,a,x,b,y} q_i \alpha_{abxy} tr(\hat{E}_{a|x} |i\rangle \langle i|)tr(\hat{b}(a|xy)). \quad (A1)$$

Note that there always exists a state $|k\rangle$ in the eigenbasis for which

$$\sum_{a,x,b,y} \alpha_{abxy} tr(\hat{E}_{a|x} |k\rangle \langle k|)tr(\hat{b}(a|xy)) \geq (A2)$$

for all $|j\rangle$. Note further that as we assume the optimal strategy one can choose wlog that $q_k \geq q_j$. This is due to the fact that if $q_k < q_j$ for some $|j\rangle$ for which the inequality in Eq. (A2) is strict one could apply a unitary exchanging $|k\rangle$ and $|j\rangle$ before and after the supposedly optimal measurements, and obtain a higher value for $R$ which contradicts our assumption that we are implementing the optimal protocol. In case the inequality is an equality we can simply relabel $|k\rangle$ to obtain $q_k \geq q_j$.

It then remains to show that by increasing the purity it is possible to increase the maximal value of $R$. Let us first consider the case that the inequality in Eq. (A2) is strict for at least one $|j\rangle$ which we will denote by $|l\rangle$. Then for any purity $Q > P$ one can find a value $\epsilon > 0$ such that $Q = (q_k + \epsilon)^2 + (q_l - \epsilon)^2 + \sum_{i \neq k,l} q_i^2$, i.e. $\epsilon = \frac{q_l - q_k}{\sqrt{2(2(\epsilon - P) + (q_l - q_k)^2)}}$. We will then use the notation $\tilde{q}_i = q_i$ for $i \notin \{k,l\}$, $\tilde{q}_k = q_k + \epsilon$ and $\tilde{q}_l = q_l - \epsilon$. It is then straightforward to see that choosing the same effects and imposing the same post-measurement states as before (e.g. by considering some measure-and-prepare channel) one obtains that

$$\sum_{a,x,b,y,i} \tilde{q}_i \alpha_{abxy} tr(\hat{E}_{a|x} |i\rangle \langle i|)tr(\hat{b}(a|xy)) > R(P). \quad (A3)$$

Hence, we have shown that for any purity $Q > P$ there exists a strategy (measurements) that allow to exceed the maximal attainable value $R(P)$ in case inequality (A2) is strict for at least one $|j\rangle$. Note that in case the inequality is an equality for the whole eigenbasis it can be easily seen that this implies that for any purity (even with the identity) the value $R(P)$ can be attained. Note further that this implies that for any purity $Q < P$ the optimal strategy has the property that for the whole eigenbasis one obtains an equality as otherwise the maximal attainable value of $R$ has to strictly increase with increasing purity as we just have shown. However, this implies that also with higher purity this value is attainable and therefore it has to hold that in this case for all $Q < P$ we have that $R(Q) = R(P)$. Increasing now $P$ one obtains that either the maximal attainable value remains constant or starts to strictly increase. In any case we have that the maximal attainable value of $R$ is monotonically increasing as a function of the purity. Hence, in case it is not constant for all purities $R$ can be used to obtain lower bounds on the purity. It is obvious that for any dimension $d$ there exists some quantity $R$ whose maximum for given purity does not remain constant for all purities.

As an example consider $B_2$ for which one can show that for the maximally mixed state the maximum is upper bounded by max[3, 4(1 − 1/d)] but the maximal value for a pure state corresponds for $d \geq 3$ to 4. This implies that also for higher dimensions the maximal attainable value of $B_1$ is strictly increasing with increasing purity. In order to see the upper bound on $B_1$ for the maximally mixed state note first that one can use an analogous argumentation to before to show that for fixed purity of the initial state either the maximal attainable value of $B_1$ is strictly increasing as a function of the purity of the post-measurement states or it remains constant. In any case, one can choose the optimal post-measurement states to be pure. As then there are only two pure post-measurement states appearing in the quantity this implies that only a two-dimensional subspace is relevant for the measurements in the second time step. Moreover, considering the first time step it is then straightforward to see that in order to obtain the maximum the diagonal terms in the effects for outcome "+" should be one in the orthogonal complement to this subspace and terms mixing the qubit subspace and its complement are chosen to be zero (in order to not introduce further constraints on the two-dimensional subspace due to positivity). We then use that one can parametrize the restriction of the effects to the two-dimensional subspace and the states as in $[12]$. That is one can use for such effects the parametrization $\hat{E}_{a|x} = a_i (|1\rangle \langle 1| + \sigma \cdot c_i) + |1\rangle \langle 1|_2$ where $|c_i\rangle \in R^3$, $|c_i\rangle = 1$, $0 \leq a_i \leq 1/(1 + b_i)$, $0 \leq b_i \leq 1$, $|1\rangle$ denotes the $x$-dimensional identity and $\sigma$ the vector of Pauli matrices (the identity) in the qubit subspace, respectively. Using then that the initial state is maximally mixed one can show analogously to $[12]$ that the maximum of $B_1$ is smaller or equal to min[3, 4(1 − 1/d)] or the effects are proportional to a projector. Considering then projective effects and the optimal choice of post-measurement states as in $[12]$ the quantity depends on one remaining
parameter, the angle between the Bloch vectors in the restriction to the two-dimensional subspace of the two measurements. It is then straightforward to see that the maximum attainable value with projective effects is given by $4(1 - 1/d)$. In summary, we have shown that for the maximally mixed state it is not possible to exceed $\max[3, 4(1 - 1/d)]$. In particular, for $d \geq 4$ we have that $4(1 - 1/d) \geq 3$ and in this case the bound can be reached. For pure initial states one can attain a value of 4 in case $d \geq 3$ (see [43]). Hence, we have that the maximal attainable value $B_1$ is not constant but due to the argumentation above strictly increasing with increasing purity. This concludes the proof that temporal correlations can be used to build witnesses for the purity of $d$-dimensional states.

Appendix B: Proof of Theorem 2

In this appendix we will show first that $B_1(p, w_{+0}, w_{+1})$ (as defined in the main text and below) is monotonically increasing as a function of $w_{+1}$ (and therefore also $\mathcal{W}_{+1}$). Moreover, we will prove Theorem 2.

Recall that $B_1(p, w_{+0}, w_{+1})$ is the maximal value for $B_1$ that is attainable with arbitrary (time-independent) measurements for a given purity $\mathcal{P} = 1/2(1 + p^2)$ of the initial state and fixed purity of the states that are measured at the second time step $\mathcal{W}_{+1} = 1/2(1 + w_{+1}^2)$ if in the first time step measurement $i$ is performed and outcome "+" is obtained. We will show that this function is monotonically increasing as a function of $\mathcal{W}_{+1}$ (assuming that all other parameters are fixed but arbitrary).

In order to do so we parametrize the effects via $\mathcal{E}_{+1} = p_x \mathbf{1} + q_x \vec{v}_x \cdot \vec{\sigma}$ and $\mathcal{E}_{-1} = \mathbf{1} - \mathcal{E}_{+1}$ for $x \in \{0, 1\}$ with $0 \leq q_x \leq p_x \leq 1 - q_x$, $\vec{v}_x \in \mathbb{R}^3$, $|\vec{v}_x| = 1$ and $\vec{\sigma}$ is a vector containing the Pauli matrices. As mentioned in the main part of the manuscript one can use the Bloch decomposition to parametrize states with fixed purity, i.e.

$$\rho = 1/2(\mathbf{1} + w \vec{\alpha} \cdot \vec{\sigma}), \quad (B1)$$

and the purity $\mathcal{W}$ is related to the length of the Bloch vector $w$ via

$$\mathcal{W} = 1/2(1 + w^2). \quad (B2)$$

Using this parametrization for the states one can analogously as in [42] determine the initial and post-measurement states that maximize $B_1$ for projective effects and purities. For this choice of states (and arbitrary effects) it can be easily seen that $B_1$ is monotonically increasing as function of $w_{+1}$ by showing that $dB_1/dw_{+1} \geq 0$ and therefore it is also a monotonically increasing function of $\mathcal{W}_{+1}$. In particular, we have that

$$B_1(p, w_{\text{max}}, w_{\text{max}}) \geq B_1(p, w_{+0}, w_{+1}),$$

where $w_{\text{max}} = \max_{x \in \{0, 1\}} w_{+i}$.

In the following we will use the notation $B_1(p, w) \equiv B_1(p, w, w)$. We will next show Theorem 2. In order to improve readability we repeat the theorem here.

**Theorem 2.** Let $\mathcal{P}$ be the purity of the initial state and $\mathcal{W}$ the purity of the post-measurement states that occur for measurement $i \in \{0, 1\}$ observing outcome "+". Then for a two-dimensional system the maximal value of $B_1$, $B_1(p, w)$, that can be obtained for arbitrary initial states and measurements that respect these constraints on the purities, is given by

$$B_1(p, w) = \begin{cases} 2 & 0 \leq w \leq \frac{1-p}{3+p} \\ \frac{1-p}{4} & \frac{1-p}{3+p} < w \leq 1 \end{cases}$$

where $w = \sqrt{2\mathcal{W} - 1}$ and $p = \sqrt{2\mathcal{P} - 1}$ are the length of the Bloch vector for the respective purity.

**Proof.** Note first that by deterministically assigning outcome "+" for both measurements independent of the state that is measured one obtains that $B_1 = 2$. Moreover, by using the following protocol one can obtain $B_1 = 1 + \frac{1-p}{(1+p)(1+p)}$. Let the initial state have a Bloch vector of length $p$ pointing in z-direction, i.e. in Eq. (B1) we have that $\vec{\alpha} = (0, 0, 1)$. One of the measurement is chosen to be of the form that one deterministically announces "+" and prepares the state with Bloch vector pointing in -z-direction, i.e. $\vec{\alpha} = (0, 0, -1)$, and of length $w$. The other measurement performs a projective measurement in the computational basis $1/2(\mathbf{1} \pm \sigma_z)$ with associated outcome "±" and then prepares the state with $\vec{\alpha} = (0, 0, 1)$ and length $w$. Hence, the values for $B_1$ given in the theorem above are attainable. Moreover, note that $2 \geq 1 + \frac{1+p}{(1+p)(1+p)}$ if and only if $w \leq \frac{1-p}{3+p}$. It remains to show that $B_1$ for given $p$ and $w$ cannot exceed $\max[2, 1 + \frac{1+w}{(1+p)(1+p)}]$. In order to do so, we note first that it can be easily seen using the same argumentation as in [42] that either $B_1(p, w) \leq 2$ or for both measurements the effects for outcome "−" are proportional to projectors. Denoting this proportionality factor for measurement $i$ by $p_i$ and considering the points where the gradient with respect to these two parameters (assuming all other parameters to be fixed but arbitrary) vanishes, we obtain that

$$\sum_i p_i \frac{\partial B_1}{\partial p_i} = 0. \quad (B3)$$

This is equivalent to

$$B_1 = \frac{1}{2} [p(+0) + p(+1) + p(|-| + 00) + p(-| + 01) + p(+| + 11) + p(-| + 10)], \quad (B4)$$

where we used that one can write $p(+b|xy) = p(+|x)p(b| + xy)$. By maximizing the right hand side
of this equation one can obtain an upper bound on $B_1$ at
the points where the gradient vanishes. Note first that
the expression is a linear function in the parameters $p_i$
and therefore is maximal at one of the boundary points
$p_i = 0$ or $p_i = 1$. If $p_0 = p_1 = 0$ then independent of
the measured states outcome "+" never occurs and therefore
the right hand side is upper bounded by two. In case
$p_0 = p_1 = 1$ the effects are projective and choosing the
optimal initial and post-measurement states analogous to
$[42]$ we get for the right hand side
\[\frac{1}{2}[6 + 2w\sqrt{2 - 2x} + p\sqrt{2 + 2x}], \quad (B5)\]
where $x$ corresponds to the angle between the Bloch vec-
tors of the effects for outcome "+" of the two measure-
ments. One can easily show that this expression is maxi-
imized for the point where the derivative with respect to
$x$ vanishes (and not at the boundary given by $x \in \{\pm 1\}$),
i.e. $x = (p^2 - 4w^2)/(p^2 + 4w^2)$. This results in a max-
imal value for the right hand side that is strictly smaller than
$1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4}$ for all possible values of $p$ and $w$.
It remains then to consider $p_0 = 0$ and $p_1 = 1$ as Eq.
$[B4]$ is symmetric with respect to the exchange of mea-
surement 0 and 1. It can be easily seen that in this case
the right hand side of Eq. $(B4)$ is at most
\[\frac{1}{2}[3 + \frac{1 + p}{2} + w] \leq 1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4}. \quad (B6)\]
In summary we have seen that for the points where
the gradient with respect to $p_i$ vanishes $B_1 \leq 2$ or $B_1 \leq 1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4}$ for the given purities which
implies in particular that $B_1 \leq \max(2, 1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4})$. In order to prove the theorem it therefore remains to show
that this upper bound also holds true at the boundary
of the domain $0 \leq p_i \leq 1$, i.e. the effect for one of
the measurements is either projective [case A] or the iden-
tity [case B]. Note that $B_1$ is symmetric regarding the
exchange of the measurements. Let us first discuss case
A and choose without loss of generality $p_1 = 1$, i.e.
measurement 1 is projective. At the points where the deriva-
tive with respect to $p_0$ vanishes one obtains that
\[B_1 = \{p(+|0) - 1)[1 - p(|+\rangle + 00\rangle)] + 1 + p(-|0) + p(+|1)p(+|11)\}
\[\leq 1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4}. \quad (B7)\]
for all $p$ and $w$ if $p_1 = 1$. It remains to consider for
case A the boundary points $p_0 = 0$ and $p_0 = 1$. The
case $p_0 = 0$ corresponds to a deterministic assignment
of outcome "+" and is included in case B. Choosing
the optimal states for the measurements with $p_0 = p_1 = 1$
and an angle between the Bloch vectors of the different
measurements denoted as before by $x$ one obtains that
in this case
\[\frac{1}{4}(2 + w\sqrt{2 - 2x})(2 + p\sqrt{2 + 2x}). \quad (B8)\]
It can be shown that at the critical points this function
is smaller or equal to $1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4}$ and therefore
with projective effects one cannot exceed this value. We
will proceed with case B and choose without loss of gen-
erality $p_0 = 0$. It is then immediate to see that the Bloch
vectors of the optimal states have to be chosen parallel
or antiparallel to the Bloch vector of measurement 1. For
this choice of states and measurements one obtains that
\[B_1 = \frac{1}{4}[8 + (1 - p)(1 - w)p_1^2 + 2p_1(-1 + p + 2w)]. \quad (B9)\]
It can be checked that for the boundary points $p_1 = 0$
and $p_1 = 1$ this implies that $B_1 = 2$ and $B_1 = 1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4}$. Moreover, it can be easily seen that
the point where the derivative with respect to $p_1$ vanishes
corresponds to a minimum. In summary, this concludes
the proof that $B_1$ for given length of the Bloch vectors
of the states, $w$ and $p$, is upper bounded by max$(2, 1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4})$. Recall that this bound is tight and
that $2 \geq 1 + \frac{1 + w}{2} + \frac{(1 + p)(1 + w)}{4}$ if and only if $w \leq \frac{1 - p}{4 + p}$,
which proves the theorem. \[\square\]

Appendix C: Proof of the upper bound on the concurrence based on the purity of a subsystem

It should be noted that the upper bound on the concurrence
given by $C(\rho_{AB}) \leq \min_{\chi \in \{A, B\}} \sqrt{2[1 - \text{tr}(\rho_{\chi}^2)]}$
has already been proven for arbitrary bipartite $d$-
dimension systems in [17]. For the sake of completeness
we provide here a (alternative but similar) proof for two-
qubit states.

Proof. We will use in the following that in the two-
qubit case it has been proven in [39] that for any $p$
there exists some decomposition into pure states, $\rho = \sum_{i=1}^r p_i |\phi_i\rangle \langle \phi_i|$, such that $C(\rho) = C(|\phi_i\rangle)$ for all $i \in \{1,\ldots,r\}$. Moreover, recall that it holds for the pure
states $|\phi_i\rangle$ that $C(|\phi_i\rangle) = \sqrt{2[1 - \text{tr}(|\phi_i\rangle^2)]}$ with $\rho_A = \text{tr}_B(|\phi_i\rangle \langle \phi_i|)$. Note that due to $C(|\phi_i\rangle) = C(|\phi_j\rangle)$ we have therefore
\[\text{tr}(|\phi_i\rangle^2) = \text{tr}(|\phi_A\rangle^2) \equiv \tilde{C}(\rho). \quad (C1)\]
From this equation it follows that
\[\text{tr}(|\phi_i\rangle^2) = \sum_{i,j} p_i p_j \text{tr}(|\phi_A\rangle^2 |\phi_B\rangle^2) \quad (C2)\]
\[\leq \sum_{i,j} p_i p_j \sqrt{\text{tr}(|\phi_A\rangle^2)^2 \sqrt{\text{tr}(|\phi_A\rangle^2)^2}}
\[= \sum_{i,j} p_i p_j \text{tr}(|\phi_A\rangle^2)^2 = \tilde{C}(\rho). \quad (C3)\]
The inequality arises from the Cauchy-Schwarz inequality (using the Hilbert-Schmidt inner product for each
summand) and then we use Eq. (C1) and $\sum p_i = 1$. Hence, we have that

$$C(\rho) = C(\{\phi_i\}) = \sqrt{2[1 - C(\rho)]} \leq \sqrt{2[1 - \text{tr}[\rho^A]^2]}.$$  

(C3)

One can show analogously that the bound also holds true for $\rho_B$ which proves the statement.

\[\square\]

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[45] The observables that one needs to measure in order to obtain the bounds in Eqs. (2) and (3) are local with respect to the splitting $A_i$ of copy $A$. For other copies $B_1$ and/or $B_2$ of copy $A$, the effects for each measurement can be set to zero.

[46] If the observable $O$ is defined on the entire system, the expected value of $O$ is equal to the trace of $O$ in the density matrix.

[47] For the observable $O$ defined on the entire system, the expected value of $O$ is equal to the trace of $O$ in the density matrix.

[48] In [42] we argued that either the maximum of $f_{A_i}$ is smaller or equal than 3 or the effects for each measurement corresponding to outcome "-" have rank 1. Examining the points where the derivative with respect to $c_i$ vanishes more closely, it can be easily seen that $B_1 \leq 2$ at those points for any given states.