All pure bipartite entangled states can be semi-self-tested with only one measurement setting on each party

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It has been known that all bipartite pure quantum states can be self-tested, i.e., any such state can be certified completely by initially measuring both subsystems of this state by proper local quantum measurements and subsequently verifying that the correlation between the measurement choices and the outcomes satisfies a specific condition. In such a protocol, a key feature is that the conclusion can still be reliable even if involved quantum measurements are untrusted, where quantum nonlocality is crucial and plays a central role, and this means that each party has to conduct at least two different quantum measurements to produce a desirable correlation. Here, we prove that when the underlying Hilbert space dimension is known beforehand, an arbitrary $d \times d$ bipartite pure state can be certified completely (up to local unitary transformations) by a certain correlation generated by a single measurement setting on each party, where each measurement yields only 3d outcomes. Notably, our protocols do not involve any quantum nonlocality. We believe that our result may provide us a remarkable convenience when certifying bipartite pure quantum states in quantum labs.

I. INTRODUCTION

In quantum physics and quantum information processing tasks, characterizing unknown quantum states is a fundamental problem. For this, a possible approach that one can take is quantum state tomography (QST), which aims to completely reconstruct the density matrices of target quantum states by performing tomographically complete quantum measurements on these states and then analyzing the outcome statistics [1, 2]. However, QST suffers from two obvious drawbacks. First, it is extremely costly and only feasible for small-scale quantum systems. Second, in order to obtain reliable results one has to make sure that the involved quantum measurements are conducted precisely, which is quite challenging due to limited precision of quantum operations and the existence of quantum noise and decoherence.

When characterizing unknown quantum states, it will be desirable to minimize the reliance on the physical descriptions of quantum operations. Typical schemes that operate on minimal physical assumptions are device-independent quantum protocols that were first introduced in the area of quantum key distribution [3–5], where one can make various nontrivial and reliable characterizations for unknown quantum states based only on the quantum nonlocality revealed by the outcome statistics produced by measuring these quantum states locally. To illustrate, consider a bipartite quantum state shared between Alice and Bob. Each party possesses a set of measurement devices, and they pick up these devices randomly to measure the subsystems they hold respectively. By repeating the procedure many times and recording all the outcome statistics, one can find out the correlation between the choices of measurement devices and the measurement outcomes, which may exhibit quantum nonlocality. If the observed quantum nonlocality is strong enough, it is possible to characterize the target state safely even if the measurement devices cannot be trusted [6–11].

An extreme scenario of device-independent quantum protocol is quantum self-testing. In Ref.[12] (see also Ref.[13]), Mayers and Yao found that when a quantum state violates the Clauser-Horne-Shimony-Holt (CHSH) inequality maximally [14], both the quantum state itself and the associated quantum measurements can be completely determined, up to local isometries. The phenomenon of self-testing is very surprising and valuable. On the one hand, it is well-known that a typical n-qubit unknown quantum system needs a density matrix of an exponential size to characterize completely, but in self-testing a single classical quantity on Bell inequality violation can certify the underlying quantum state. On the other hand, self-testing enables reliable benchmarking of the quality of entangled quantum states, even if the involved quantum measurements are untrustworthy. This is particularly useful in many quantum information processing tasks [3–5]. After the phenomenon of quantum self-testing was discovered, various specific bipartite and multipartite pure states were also shown to be self-testable [15–24].

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Recently, a seminal work in Ref.[25] proved that all bipartite pure states can be self-tested. Furthermore, in another breakthrough on quantum self-testing, by examining correlations generated by quantum networks it has also been proved that all multipartite pure states can be self-tested [26]. These remarkable discoveries imply that the possibility of self-testing is a general feature for pure quantum states. On the other hand, it has been known that mixed quantum states cannot be self-tested, as any correlation produced by a mixed state can always be generated by another pure state [11].

Fundamentally, the crucial concept that enables quantum self-testing is quantum nonlocality, which means that when self-testing a bipartite pure quantum state, each party must involve at least two measurement settings [27]. Indeed, if each party has only one measurement setting, it is impossible to exhibit quantum nonlocality at all, and furthermore, the resulting correlation can always be produced classically [28], making quantum self-testing impossible. In such a situation, a profound question arises: Is quantum nonlocality a necessary condition for determining a quantum state based only on the observed correlation? Surprisingly, as we shall demonstrate, if the underlying Hilbert space dimension is known beforehand, any bipartite pure state can be certified completely (up to local transformations) based only on a certain correlation produced by measuring the state with only one measurement setting on each party. We achieve this by exploiting a close relationship between the mathematical structure of correlations generated by local quantum measurements and that of positive semidefinite factorizations, a concept originated from optimization theory [29–31].

We call such a phenomenon semi-self-testing. We stress that when semi-self-testing a $d \times d$ bipartite quantum pure state, the only local quantum measurement conducted by each party has only 3d outcomes, implying that they are far from tomographically complete. We believe the discovery in the current manuscript not only helps us to gain a better understanding of the essence of quantum self-testing, but also provides us a potential new approach to efficiently certify crucial quantum states in many quantum information processing tasks.

II. THE SETTING

Suppose $\rho \in \mathcal{H}_A \otimes \mathcal{H}_B$ is a $d \times d$ bipartite quantum state shared by Alice and Bob. Then both of them measure the corresponding subsystem by a local quantum measurement, where the POVM operators for Alice are $\{A_x\}$, and those for Bob are $\{B_y\}$. Here $x, y \in [m] \equiv \{1, 2, ..., m\}$ and $\sum_x A_x = \sum_y B_y = I_d$, where I_d is the d-dimensional identity operator. We denote the probability that Alice obtains the outcome x and Bob obtains the outcome y by P_{xy} , i.e.,

$$P_{xy} = \operatorname{tr}(\rho(A_x \otimes B_y)). \tag{1}$$

We call the $m \times m$ matrix $P = [P_{xy}]$ a classical correlation generated by measuring ρ with the POVMs $\{A_x\}$ and $\{B_y\}$.

It turns out that there is a close relation between ρ and the so-called positive semidefinite factorizations (PSD factorizations) of P [31]. Suppose two set of $r \times r$ PSD matrices $\{C_x\}$ and $\{D_y\}$ satisfy that $P_{xy} = \operatorname{tr}(C_x D_y)$ for any $x, y \in [m]$, we say $\{C_x\}$ and $\{D_y\}$ form a PSD factorizations for P, and the PSD rank of P is r if the size of such $\{C_x\}$ and $\{D_y\}$ is minimal. Particularly, if $\{C_x\}$ and $\{D_y\}$ also satisfy that $\sum_{x=1}^m C_x = \sum_{y=1}^m D_y = \Lambda$, where Λ is a diagonal PSD matrix, we say $\{C_x\}$ and $\{D_y\}$ form a canonical form of PSD factorization for P. The following conclusion shows that every normal PSD factorization corresponds to a canonical form.

Proposition 1. Suppose $\{C_x\}$ and $\{D_y\}$ form a PSD factorization for a correlation P, where $S_C = \sum_x C_x$ and $S_D = \sum_y D_y$ are full rank. Then this factorization corresponds to a normal form of PSD factorization where the diagonal entries of Λ are the eigenvalues of $\left(S_C^{1/2}S_DS_C^{1/2}\right)^{1/2}$.

Proof. Consider

$$\begin{split} C_x' &= \left(S_C^{1/2} S_D S_C^{1/2}\right)^{1/4} \left(S_C^{-1/2} C_x S_C^{-1/2}\right) \left(S_C^{1/2} S_D S_C^{1/2}\right)^{1/4}, \\ D_y' &= \left(S_C^{1/2} S_D S_C^{1/2}\right)^{-1/4} \left(S_C^{1/2} D_y S_C^{1/2}\right) \left(S_C^{1/2} S_D S_C^{1/2}\right)^{-1/4}. \end{split}$$

It can be verified that

$$\operatorname{tr}(C'_x D'_y) = \operatorname{tr}(C_x D_y),$$

$$\sum_x C'_x = \sum_y D'_y = \left(S_C^{1/2} S_D S_C^{1/2}\right)^{1/2}.$$

Suppose a unitary matrix U can diagonalize $\left(S_C^{1/2}S_DS_C^{1/2}\right)^{1/2}$, then $\{UC_x'U^{\dagger}\}$ and $\{UD_y'U^{\dagger}\}$ form a normal form of PSD factorization for P, where the diagonal entries of Λ are the eigenvalues of $\left(S_C^{1/2}S_DS_C^{1/2}\right)^{1/2}$.

It has been known that if ρ generates P, then there exists a pure state $|\psi\rangle$ in $\mathcal{H}_{A_1} \otimes \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_{B_1}$ such that it is a purification for both ρ and $\sigma = \sum_{x,y=1}^{m} P_{xy} \cdot |x\rangle \langle x| \otimes |y\rangle \langle y| \in \mathcal{H}_A \otimes \mathcal{H}_B$ [31]. In addition, suppose the Schmidt rank of $|\psi\rangle$ with respect to the partition $AA_1|BB_1$ is r, and the Schmidt coefficients are $\sqrt{\lambda_i}$, $i \in [r]$, then P has a canonical form of PSD factorization, denoted $\{C_k\}$ and $\{D_l\}$, such that $\Lambda = \sum_{k=1}^m C_k = \sum_{l=1}^m D_l = \operatorname{diag}(\sqrt{\lambda_1}, ..., \sqrt{\lambda_r})$, where $\operatorname{diag}(a_1, a_2, ..., a_n)$ is a $d \times d$ diagonal matrix with the diagonal entries a_i 's [32].

A CORRELATION THAT SEMI-SELF-TESTS THE MAXIMALLY ENTANGLED STATE

Let $\vec{e} \in \mathbb{R}^d$ be the d-dimensional column vector with all entries equal to one. Consider the following $2d \times 2d$ classical correlation specified in block matrix form:

$$P = \frac{1}{d(d+1)^2} \begin{pmatrix} d^2 I_d & \vec{e}\vec{e}^T \\ \vec{e}\vec{e}^T & I_d \end{pmatrix}. \tag{2}$$

We now are ready to introduce the first main result of the current paper.

Theorem 2. If Alice and Bob can generate P by locally measuring a bipartite $d \times d$ quantum state ρ with the POVMs $\{A_x\}$ and $\{B_u\}$, then ρ must be a $d \times d$ maximally entangled pure state.

To prove this conclusion, we need to examine all possible PSD factorizations for P. Given a PSD factorization for

P, we denote the matrices therein by $\{C_1, C_2, ..., C_{2d}\}$ and $\{D_1, D_2, ..., D_{2d}\}$. We first consider the lower right submatrix $\frac{1}{d(d+1)^2}I_d$ in P. It can be verified that this implies that for $x, y \in [d]$, C_x and D_y must be rank-1, i.e., $C_{d+x} = a_x |\alpha_x\rangle \langle \alpha_x'|$ and $D_{d+y} = b_y |\beta_y\rangle \langle \beta_y|$ for certain pure states $|\alpha_x\rangle$ and $|\beta_y\rangle$, and positive real number a_x and b_y . Furthermore, the vector set $\{|\alpha_x\rangle\}(x \in [d])$ is linearly independent, and similar for $\{|\beta_u\rangle\}(y\in[d])$. To see why this is the case, for each $x\in[d]$ we pick unit vectors $a_x\in\mathrm{range}(C_{d+x})$ and $b_x \in \text{range}(D_{d+x})$ such that $\langle a_x, b_x \rangle \neq 0$; this is possible since $\text{tr}(C_{d+x}D_{d+x}) > 0$, where range(A) is the subspace consisting of all linear combinations of the eigenvectors of A with nonzero eigenvalues. Suppose the vectors b_x are linearly dependent; that is, without loss of generality,

$$b_1 = \sum_{x=2}^d \alpha_x b_x,$$

where α_x are complex scalars. Then

$$0 \neq \langle a_1, b_1 \rangle = \sum_{x=2}^{d} \alpha_x \langle a_1, b_x \rangle = 0,$$

which is impossible. This gives

$$rank(D_{d+2} + \cdots + D_{2d}) \ge dim(span\{b_2, \cdots, b_d\}) = d - 1,$$

where rank(A) is the rank of the matrix A, $\dim(S)$ is the dimension of a vector space S, and span $\{b_2, \dots, b_d\}$ is the vector space consisting of all linear combinations of the vectors b_2, \dots, b_d . Since $\operatorname{tr}(C_{d+1}(D_{d+2} + \dots + D_{2d}) = 0$, we have $\operatorname{rank}(C_{d+1}) \leq 1$, hence $\operatorname{rank}(C_{d+1}) = 1$ due to $C_{d+1} \neq 0$. By symmetry we have $\operatorname{rank}(C_{d+x}) = 1$ for all $x \in [d]$,

and by swapping the roles of C_{d+x} and D_{d+y} we get $\operatorname{rank}(D_{d+y}) = 1$ for all $y \in [d]$. Therefore, one can find an invertible matrix H such that $HC_{d+x}H^{\dagger} = \frac{1}{\sqrt{d(d+1)}}|x-1\rangle\langle x-1|$, where $x \in [d]$ and $\{|i\rangle\}(0 \le i \le d-1)$ are the computational basis states. For any $x,y \in [2d]$, we let $C'_x = HC_xH^{\dagger}$ and $D'_y = (H^{\dagger})^{-1}D_yH^{-1}$, then $\{C'_x\}$ and $\{D'_y\}$ also form a PSD factorization for P. When focusing on $y \in [d]$, by direct calculations we can see that $D'_{d+y} = \frac{1}{\sqrt{d(d+1)}} |y-1\rangle \langle y-1|$.

Similarly, for any $x, y \in [d]$ the matrices C'_x and D'_y must be of rank 1 since they have to produce the submatrix $\frac{d^2}{d(d+1)^2}I_d \text{ of } P. \text{ Additionally, for any } x,y \in [d] \text{ the diagonals of } C_x' \text{ and } D_y' \text{ are all } \frac{1}{\sqrt{d}(d+1)} \text{ (from the two submatrices } \frac{1}{d(d+1)^2}\vec{e}\vec{e}^T \text{ of } P), \text{ hence all entries of } C_x' \text{ and } D_y' \text{ have norms at most } \frac{1}{\sqrt{d}(d+1)}. \text{ For any } x \in [d], \text{ since } \frac{d}{(d+1)^2} = \frac{1}{d(d+1)^2}\vec{e}^T \text{ of } P$ $\operatorname{tr}(C_x'D_x') \leq \sqrt{\operatorname{tr}(C_x'^2)\operatorname{tr}(D_x'^2)} = \frac{d}{(d+1)^2}$ with the equality holding if and only if C_x' is proportional to D_x' , we have $C_x' = D_x'$. Thus the constraint $\operatorname{tr}(C_x'D_y') = \frac{d}{(d+1)^2}\delta_{xy}$ implies that $\sum_{x=1}^d C_x' = \sum_{y=1}^d D_y' = \frac{\sqrt{d}}{d+1}I_d$.

In fact, for any $x,y\in [d]$ if setting $C_x'=D_x'=\frac{\sqrt{d}}{d+1}|\gamma_x\rangle\langle\gamma_x|$ where $|\gamma_x\rangle$ is the x-th column of the $d\times d$ quantum Fourier transform matrix, and then combining the above choices of $\{C_{d+x}'\}$ and $\{D_{d+y}'\}$ together, one can verify that $\{C_x'\}$ and $\{D_y'\}$ do form a valid PSD factorization for P. Furthermore, we also have that $\sum_{x=1}^{2d} C_x' = \sum_{y=1}^{2d} D_y' = \frac{1}{\sqrt{d}}I_d$, implying that $\{C'_x\}$ and $\{D'_y\}$ form a canonical form of PSD factorization for P. Interestingly, we also observe the following key fact.

Lemma 3. The canonical form of PSD factorization for P is unique.

Proof. Suppose $\{C_x''\}$ and $\{D_y''\}$ is another canonical form of PSD factorization for P, and $\sum_{x=1}^{2d} C_x'' = \sum_{y=1}^{2d} D_y'' = \Lambda'$, where Λ' is a diagonal PSD matrix. Then according to our discussion above, all C_x'' and D_y'' must be rank-1, and there exists an invertible matrix M such that for each $x \in [d]$, $MC''_{d+x}M^{\dagger}$ has the form of $\frac{1}{\sqrt{d(d+1)}}|x-1\rangle\langle x-1|$. Again based on our above discussion, for $x,y \in [2d]$, $\{MC_x''M^{\dagger}\}$ and $\{(M^{\dagger})^{-1}D_y''(M)^{-1}\}$ will be the canonical form of PSD factorization $\{C_x'\}$ and $\{D_y'\}$ introduced above. That is, $\sum_{x=1}^{2d} M C_x'' M^{\dagger} = M \Lambda' M^{\dagger} = \frac{1}{\sqrt{d}} I_d$, and $\sum_{x=1}^{2d} (M^{\dagger})^{-1} C_x'' M^{-1} = (M^{\dagger})^{-1} \Lambda' M^{-1} = \frac{1}{\sqrt{d}} I_d$. This means that $M M^{\dagger} = I_d$, i.e., $\Lambda' = M^{\dagger} \cdot \frac{1}{\sqrt{d}} I_d \cdot M = \frac{1}{\sqrt{d}} I_d$.

Note that ρ can be a mixed state, and if this is the case, Bob can purify ρ to be a pure state $|\phi\rangle$ in $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_R$ by introducing an ancillary system R. After that, Alice and Bob can generate P by measuring $|\phi\rangle$ with the POVMs $\{A_x\}$ and $\{B_y \otimes I_R\}$, where I_R is the identity operator on the system R. According to Ref.[32], we know that with respect to the partition A|BR, the Schmidt coefficients of $|\phi\rangle$ is the diagonal entries of $\frac{1}{\sqrt{d}}I_d$, i.e., $\{\frac{1}{\sqrt{d}},\frac{1}{\sqrt{d}},...,\frac{1}{\sqrt{d}}\}$. Since the ancillary system R can also be introduced by Alice, we obtain the following conclusion.

Proposition 4. $\operatorname{tr}_A(\rho) = \operatorname{tr}_B(\rho) = \frac{1}{d}I_d$.

Due to the above lemma, if we can next show that the state ρ is pure, then it must be a bipartite maximally entangled pure state. For this, we need to use the following fact.

Proposition 5. All measurement operators A_x and B_y have rank 1, where $x, y \in [2d]$.

Proof. Let $\tilde{B}_y = \operatorname{tr}_B((I_A \otimes \sqrt{B_y})\rho(I_A \otimes \sqrt{B_y}))$. Then $P_{xy} = \operatorname{tr}(A_x \tilde{B}_y) = \operatorname{tr}(\rho(A_x \otimes B_y))$. Note that \tilde{B}_y is a PSD matrix for any $y \in [2d]$, thus we can apply the technique we have utilized before to prove that rank $(A_x) = 1$ for any $x \in [2d]$. By swapping the roles of A_x and B_y we get rank $(B_y) = 1$ for all $y \in [2d]$.

Then A_x and B_y can be further characterized as below.

Proposition 6. For $i, j \in [d]$ with $i \neq j$, we have

$$A_i A_j = B_i B_j = A_{d+i} A_{d+j} = B_{d+i} B_{d+j} = 0.$$

Proof. We now show that $A_1A_2=0$, and the other cases can be proved similarly. Recall that $P_{xy}=\operatorname{tr}(\rho(A_x\otimes B_y))$, then it holds that

$$\sum_{y=1}^{2d} P_{1y} = \operatorname{tr}(\rho(A_1 \otimes I_d)) = \operatorname{tr}(\operatorname{tr}_B(\rho) \cdot A_1) = \frac{\operatorname{tr}(A_1)}{d}.$$

Combined with $\sum_{y=1}^{2d} P_{1y} = \frac{1}{d+1}$, this means that $\operatorname{tr}(A_1) = \frac{d}{d+1}$. Recall also that A_1 is rank-1, so without loss of generality we can perform local unitaries on both ρ and all POVM operators such that they still generate P and $A_1 = B_1 = \frac{d}{d+1} |0\rangle \langle 0|$. Let

$$A_2 = \frac{d}{d+1} (\alpha |0\rangle + \beta |\bar{1}\rangle) (\alpha^* \langle 0| + \beta^* \langle \bar{1}|),$$

where $|\bar{1}\rangle$ is some vector orthogonal to $|0\rangle$ and $|\alpha|^2 + |\beta|^2 = 1$. Then

$$\langle 00|\rho|00\rangle = \frac{(d+1)^2}{d^2} \text{tr}(\rho(A_1 \otimes B_1))$$

$$= \frac{1}{d},$$

$$A_2 \otimes B_1 = \frac{d^2}{(d+1)^2} \left(|\alpha|^2 |00\rangle \langle 00| + \alpha\beta^* |00\rangle \langle \bar{1}0| + \alpha^*\beta |\bar{1}0\rangle \langle 00| + |\beta|^2 |\bar{1}0\rangle \langle \bar{1}0| \right).$$

Since $\operatorname{tr}_A(\rho) = \frac{I_d}{d}$, we have

$$\begin{split} \langle 00|\rho|00\rangle + \langle \bar{1}0|\rho|\bar{1}0\rangle &= \mathrm{tr}(\rho((|0\rangle\langle 0| + |\bar{1}\rangle\langle \bar{1}|) \otimes (|0\rangle\langle 0|))) \\ &\leq \mathrm{tr}(\rho(I_d \otimes |0\rangle\langle 0|)) \\ &= \mathrm{tr}(\mathrm{tr}_A(\rho) |0\rangle\langle 0|) \\ &= \mathrm{tr}(\frac{I_d}{d} |0\rangle\langle 0|) \\ &= \frac{1}{d}. \end{split}$$

Therefore, by $\rho \ge 0$ and $\langle 00|\rho|00\rangle = \frac{1}{d}$ we have $\langle \bar{1}0|\rho|\bar{1}0\rangle = 0$, which implies that $\langle \bar{1}0|\rho|00\rangle = \langle 00|\rho|\bar{1}0\rangle = 0$. As a result, it holds that

$$0 = \operatorname{tr}(\rho(A_2 \otimes B_1))$$

$$= \frac{d^2}{(d+1)^2} |\alpha|^2 \cdot \frac{1}{d}$$

$$= \frac{d}{(d+1)^2} |\alpha|^2.$$

This implies that $\alpha = 0$ and $A_1 A_2 = 0$.

Because of the above fact, we may perform two local unitaries on each parties so that for $i \in [d]$ it holds that A_i and B_i are both proportional to $|i-1\rangle\langle i-1|$, where ρ is also adjusted accordingly. Meanwhile, using the same technique to calculate $\operatorname{tr}(A_1)$, we can obtain that $\operatorname{tr}(A_i) = \frac{d}{d+1}$ for any $i \in [d]$. Combining these two observations together, we can let $A_i = \frac{d}{d+1}|i-1\rangle\langle i-1|$ and $B_i = \frac{d}{d+1}|i-1\rangle\langle i-1|$ for any $i \in [d]$.

can let $A_i = \frac{d}{d+1} |i-1\rangle \langle i-1|$ and $B_i = \frac{d}{d+1} |i-1\rangle \langle i-1|$ for any $i \in [d]$. Lastly, since $P_{ij} = \operatorname{tr}(\rho(A_i \otimes B_j)) = 0$ for any $i \neq j \in [d]$, we have that $\operatorname{range}(\rho) \subseteq \operatorname{span}\{|00\rangle, |11\rangle, \cdots, |(d-1)(d-1)\rangle\}$. Similarly, it holds that $\langle ii|\rho|ii\rangle = \frac{1}{d}$, which also means $|\langle ii|\rho|jj\rangle| \leq \frac{1}{d}$ since ρ is a PSD matrix, here $i, j \in \{0, \cdots, d-1\}$.

Proposition 7. $|\langle i|A_{d+1}|j\rangle| = |\langle i|B_{d+1}|j\rangle| = \frac{1}{d(d+1)} \text{ for all } i, j \in \{0, \dots, d-1\}.$

Proof. For any $i \in \{0, \dots, d-1\}$ we have

$$\frac{1}{d(d+1)^2} = \operatorname{tr}(\rho(A_{i+1} \otimes B_{d+1}))$$

$$= \frac{d}{d+1} \operatorname{tr}(\rho(|i\rangle \langle i| \otimes B_{d+1}))$$

$$= \frac{d}{d+1} \sum_{jkj'k'} \langle jk|\rho|j'k'\rangle \langle j'k'| (|i\rangle \langle i| \otimes B_{d+1}) |jk\rangle$$

$$= \frac{d}{d+1} \sum_{kk'} \langle ik|\rho|ik'\rangle \langle k'|B_{d+1}|k\rangle$$

$$= \frac{d}{d+1} \cdot \frac{1}{d} \langle i|B_{d+1}|i\rangle$$

$$= \frac{1}{d+1} \cdot \langle i|B_{d+1}|i\rangle,$$

hence $\langle i|B_{d+1}|i\rangle = \frac{1}{d(d+1)}$. Since rank $(B_{d+1}) = 1$, the rest of the entries also have norms $\frac{1}{d(d+1)}$.

We now examine the (d+1, d+1)-th entry of P using the Cauchy-Schwarz inequality:

$$\begin{split} \frac{1}{d(d+1)^2} &= \operatorname{tr}(\rho(A_{d+1} \otimes B_{d+1})) \\ &= \sum_{iji'j'} \langle ij|\rho|i'j'\rangle \, \langle i'j'|A_{d+1} \otimes B_{d+1}|ij\rangle \\ &= \sum_{ii'} \langle ii|\rho|i'i'\rangle \, \langle i'|A_{d+1}|i\rangle \, \langle i'|B_{d+1}|i\rangle \\ &\leq \left(\sum_{ii'} |\langle ii|\rho|i'i'\rangle|^2\right)^{1/2} \left(\sum_{ii'} |\langle i'|A_{d+1}|i\rangle \, \langle i'|B_{d+1}|i\rangle|^2\right)^{1/2} \\ &\leq \left(d^2 \cdot d^{-2}\right)^{1/2} \left(d^2 \cdot (d(d+1))^{-4}\right)^{1/2} \\ &= \frac{1}{d(d+1)^2}. \end{split}$$

Therefore, there exists a scalar α such that

$$\langle ii|\rho|i'i'\rangle = \alpha \langle i'|A_{d+1}|i\rangle \langle i'|B_{d+1}|i\rangle.$$

This implies that $\operatorname{rank}(\rho) = 1$, hence ρ is a pure state. By $\operatorname{tr}_A(\rho) = \operatorname{tr}_B(\rho) = \frac{I_d}{d}$, we conclude that ρ is the maximally entangled state.

A CORRELATION THAT SEMI-SELF-TESTS A GENERAL BIPARTITE PURE ENTANGLED

We now generalize the techniques developed in Sec.III to show that any $d \times d$ bipartite pure entangled state $|\psi\rangle$ can be semi-self-tested. Without loss of generality, we assume that the Schmidt rank of $|\psi\rangle$ is d.

We define $\vec{z} = (z_1, z_2, ..., z_d) \in \mathbb{R}^d$ to be a d-dimensional column vector with all entries positive, and the values of its entries z_i will be fixed later. Consider the following classical correlation of size $3d \times 3d$:

$$Q = \begin{pmatrix} a \cdot P & \begin{pmatrix} \vec{e}\vec{z}^T \\ \operatorname{diag}(\vec{z}) \end{pmatrix} \\ \begin{pmatrix} \vec{z}\vec{e}^T & \operatorname{diag}(\vec{z}) \end{pmatrix} & \frac{d(d+1)^2}{a} \operatorname{diag}(\vec{z})^2 \end{pmatrix},$$
(3)

where 0 < a < 1 is a positive real number that we will pin down later, and P is the $2d \times 2d$ classical correlation defined in Eq.(2). As a classical correlation, the sum of all entries of Q must be 1, and this means that

$$a + 2(d+1)\|\vec{z}\|_1 + \frac{d(d+1)^2}{a}\|\vec{z}\|_2^2 = 1,$$

where $\|\vec{z}\|_1 = \sum_{i=1}^d z_i$ and $\|\vec{z}\|_2^2 = \sum_{i=1}^d z_i^2$. Suppose $\{C_x\}$ and $\{D_y\}$ form a canonical form of PSD factorization for Q, where $x, y \in [3d]$. Then using the same techniques as in Sec.III, one can prove that we must have that $\sum_{x=1}^{3d} C_x = \sum_{y=1}^{3d} D_y = \Lambda$, where

$$\Lambda = \operatorname{diag}(\gamma_1, \gamma_2, ..., \gamma_d),$$

and
$$\gamma_i = \sqrt{\frac{a}{d}} + \sqrt{\frac{d}{a}}(d+1) \cdot z_i$$
 for any $i \in [d]$.

This can be explained as below. First, let us first focus on the submatrix $a \cdot P$, then according to the discussions in Sec.III we know that $\{C_x\}$ and $\{D_y\}$ must be rank-1 for any $x, y \in [2d]$. In addition, for any $x, y \in [d]$, by a proper invertible matrix S we can have that $SC_{d+x}S^{\dagger} = \frac{\sqrt{a}}{\sqrt{d(d+1)}}|x-1\rangle\langle x-1|$ and $(S^{\dagger})^{-1}D_{d+y}S^{-1} = \frac{\sqrt{a}}{\sqrt{d(d+1)}}|y-1\rangle\langle y-1|$. Similarly, SC_xS^{\dagger} and $(S^{\dagger})^{-1}D_yS^{-1}$ can also be characterized accordingly for any $x, y \in [d]$. For convenience, we still denote the adjusted PSD factorizations for Q by $\{C'_x\}$ and $\{D'_y\}$, where $x, y \in [3d]$.

Next we focus on the two submatrices $\operatorname{diag}(\vec{z})$ of Q. Based on this part we can know that when $x, y \in [d]$, it holds that $C'_{2d+x} = \frac{\sqrt{d}(d+1)}{\sqrt{a}} \cdot z_x |x-1\rangle \langle x-1|$, and $D'_{2d+y} = \frac{\sqrt{d}(d+1)}{\sqrt{a}} \cdot z_y |y-1\rangle \langle y-1|$. By direct calculations, one can verify that the above choices of $\{C'_x\}$ and $\{D'_y\}$ are indeed a valid PSD factorization for Q, and what is more, it holds that

$$\sum_{x=1}^{3d} C_x' = \sum_{y=1}^{3d} D_y' = \operatorname{diag}(\gamma_1, \gamma_2, ..., \gamma_d), \tag{4}$$

where $\gamma_i = \sqrt{\frac{a}{d}} + \sqrt{\frac{d}{a}}(d+1) \cdot z_i$ for any $i \in [d]$.

Notice that for any PSD factorizations of Q, all the involved PSD matrices must be rank-1, thus the technique utilized in Lemma 3 can also be applied here, and as a result, Q has a unique canonical form of PSD factorization, which is given in Eq.(4).

We now suppose that Alice and Bob generate Q by measuring a $d \times d$ bipartite quantum state $\rho_Q \in \mathcal{H}_A \otimes \mathcal{H}_B$ with We now suppose that Alice and Bob generate Q by measuring a $a \times a$ bipartite quantum state $\rho_Q \in \mathcal{H}_A \otimes \mathcal{H}_B$ with two local POVM quantum measurements, and the operators for Alice are $\{A_x\}$, and those for Bob are $\{B_y\}$, where $x, y \in [3d]$ and $\sum_{x=1}^{3d} A_x = \sum_{y=1}^{3d} B_y = I_d$. Let $A_P = \sum_{x=1}^{2d} A_x$ and $B_P = \sum_{y=1}^{2d} B_y$ be the sum of measurement operators corresponding to the block $a \cdot P$ of Q. Since $a \cdot P$ must be generated by a $d \times d$ state and P contains submatrix of PSD rank d, we have rank $(A_P) = \operatorname{rank}(B_P) = d$; that is, both A_P and B_P are invertible. Then it can be seen that $\frac{1}{a} \cdot (A_P \otimes B_P)^{1/2} \rho_Q(A_P \otimes B_P)^{1/2}$ generates P when measured by the POVMs with the measurement operators $\{A_P^{-1/2}A_xA_P^{-1/2}\}$ and $\{B_P^{-1/2}B_yB_P^{-1/2}\}$, where $x, y \in [2d]$. By the previous section we have that $\frac{1}{a} \cdot (A_P \otimes B_P)^{1/2}\rho_Q(A_P \otimes B_P)^{1/2}$ must be pure, hence the bipartite state ρ_Q is also pure. Furthermore, the Schmidt coefficients of ρ_Q is exactly the ρ_Q 's in Eq.(4)

Schmidt coefficients of ρ_Q is exactly the γ_i 's in Eq.(4).

Therefore, suppose one wants to semi-self-test a $d \times d$ pure quantum state with the Schmidt decomposition

$$|\psi\rangle = \sum_{k=1}^{d} \sqrt{\lambda_i} |\alpha_i\rangle \otimes |\beta_i\rangle,$$
 (5)

where $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_d > 0$, and $\{|\alpha_i\rangle\}$ and $\{|\beta_i\rangle\}$ are orthonormal states for Alice and Bob respectively. Then what he/she needs to do is to set a and \vec{z} properly such that the γ_i 's in Eq.(4) are exactly the same with $\sqrt{\lambda_i}$. It can be verified that this can be achieved by letting

$$a = \frac{d}{4} \cdot \lambda_d \tag{6}$$

and

$$z_i = \frac{1}{d+1} \cdot \frac{\sqrt{\lambda_d}}{2} \left(\sqrt{\lambda_i} - \frac{1}{2} \sqrt{\lambda_d} \right) \tag{7}$$

for any $i \in [d]$.

SEMI-SELF-TESTING QUANTUM STATES WITH INEQUALITIES

For a $d \times d$ classical correlation A, we denote its entries by A_{ij} $(i, j \in [d])$. By the Cauchy-Schwarz inequality, for any $3d \times 3d$ classical correlation P it holds that

$$\sum_{x,y=1}^{3d} \sqrt{P_{xy}} \cdot \sqrt{Q_{xy}} \le 1 \tag{8}$$

and the equality holds if and only if P = Q, where Q is the classical correlation in Eq.(3), and we have utilized the relations $\sum_{x,y} P_{xy} = \sum_{x,y} Q_{xy} = 1$. Therefore, we have the following main result.

Theorem 8. If Alice and Bob generate a $3d \times 3d$ classical correlation P by locally measuring a $d \times d$ bipartite quantum state ρ with the POVMs $\{A_x\}$ and $\{B_y\}$ $(x, y \in [3d])$, and saturates the inequality in Eq.(8), then ρ must be a $d \times d$ pure state with the Schmidt coefficients $\sqrt{\lambda_i}$ $(i \in [d])$ satisfying Eqs.(6) and (7).

Lastly, we would like to point out that some $d \times d$ pure states can be semi-self-tested by classical correlations of smaller size, and such size can be as small as d+1. Since any classical correlations of size $d \times d$ can always be generated by a $d \times d$ separable state [28], d+1 is the smallest we can expect.

VI. DISCUSSION

In conclusion, we have proven that if the dimension of a bipartite quantum system is known, any pure state of this system can be semi-self-tested by a Bell experiment involving a single measurement setting on each party. Importantly, our protocol does not rely on quantum nonlocality since an entirely classical protocol is able to generate the same correlation with strictly larger dimensions. Though our protocol needs the information on underlying quantum dimension in constrast to normal quantum self-testing, our results still suggest that quantum self-testing may be much more general than what many people think, and could potentially manifest in various settings.

We stress that in order to semi-self-test a $d \times d$ bipartite pure quantum state, each quantum measurement in our protocol generates only 3d outcomes, which seems to be appealing for practical purposes. We believe that our results imply a new potential approach to certify crucial quantum states for many quantum information processing tasks in an efficient way.

Before applying our protocol in realistic quantum schemes, another important issue we have to address is how robust to noise our protocol can be. That is, if the correlation we observe in a quantum experiment is not exactly P or Q we have discussed, but very close, can we guarantee that the underlying quantum state has high fidelity with the ideal pure state that P or Q semi-self-tests? Moreover, if this is the case, can we give a useful lower bound for this fidelity based on the observed correlation? Lastly, we also expect that similar protocols can be designed to semi-self-test multipartite pure quantum state. We leave these problems for future work.

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