Quantifying non-classicality with local unitary operations

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We propose a measure of non-classical correlations in bipartite quantum states based on local unitary operations. We prove the measure is non-zero if and only if the quantum discord is non-zero; this is achieved via a new characterization of zero discord states in terms of the state's correlation matrix. Moreover, our scheme can be extended to ensure the same relationship holds even with a generalized version of quantum discord in which higher-rank projective measurements are allowed. We next derive a closed form expression for our scheme in the cases of Werner states and (2 × N)-dimensional systems. The latter reveals that for (2 × N)-dimensional states, our measure reduces to the geometric discord [Dakić et al., PRL 105, 2010]. A connection to the CHSH inequality is shown. We close with a characterization of all maximally non-classical, yet separable, (2 × N)-dimensional states of rank at most two (with respect to our measure).

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I. INTRODUCTION

One of the most intriguing aspects of quantum mechanics is quantum entanglement, which with the advent of quantum computing, was thrust into the limelight of quantum information theoretic research [1]. We now know that correlations in quantum states due to entanglement are necessary in order for pure-state quantum computation to provide exponential speedups over its classical counterpart [2]. With bipartite entanglement nowadays fairly well understood, however, attention has turned in recent years to a more general type of quantum correlation, dubbed simply non-classical correlations. Unlike entanglement, such correlations can be created via Local Operations and Classical Communication (LOCC), but nevertheless do not exist in the classical setting. Moreover, for certain mixed-state quantum computational feats, the amount of entanglement present can be small or vanishing, such as in the DQC1 model of computing [3] and the locking of classical correlations [4]. In these settings, it is rather non-classical correlations which are the conjectured resource enabling such feats (see, e.g. [5–8]). In fact, almost all quantum states possess non-classical correlations [9].

As a result, much attention has recently been devoted to the quantification of non-classical correlations (e.g., [11–23], see [24] for a survey). Here, we say a bipartite state ρ acting on Hilbert space A ⊗ B is classically correlated in A if and only if there exists an orthonormal basis { |a⟩} for A such that

\[ \rho = \sum_{i} p_{i} |a_{i}\rangle\langle a_{i}| \otimes \rho_{i} \]

for {p_{i}} a probability distribution and ρ_{i} density operators. To quantify “how far” ρ is from the form above, a number of non-classicality measures, including perhaps the best-known such measure, the quantum discord [25,26], ask the question of how drastically a bipartite quantum state is disturbed under local measurement on A. In this paper, we take a different approach to the problem. We ask: Can disturbance of a bipartite system under local unitary operations be used to quantify non-classical correlations?

It turns out that not only is the answer to this question yes, but that in fact for (2 × N)-dimensional systems, the measure we construct coincides with the geometric quantum discord [21], a scheme based again on local measurements. Our measure is defined as follows. Given a bipartite quantum state ρ and unitary U_{A} acting on Hilbert spaces A ⊗ B and A with dimensions MN and M, respectively, define

\[ D(\rho, U_{A}) := \frac{1}{\sqrt{2}} \left\| \rho - (U_{A} \otimes I_{B}) \rho (U_{A}^{\dagger} \otimes I_{B}) \right\|_{F}, \]

(1)

where the Frobenius norm \( \| A \|_{F} = \sqrt{\text{Tr} A^{\dagger}A} \) is used due to its simple calculation. Then, consider the set of unitary operators whose eigenvalues are some permutation of the M-th roots of unity, i.e. whose vector of eigenvalues equals \( \pi v \) for \( \pi \in S_{M} \) some permutation and \( v_{k} = e^{2\pi k i / M} \) for \( 1 \leq k \leq M \). We call such operators Root-of-Unity (RU) unitaries. They include, for example, the Pauli X, Y, and Z matrices. Then, letting RU(A) denote the set of RU unitaries acting on A, we define our measure as:

\[ D(\rho) := \min_{U_{A} \in \text{RU}(A)} D(\rho, U_{A}). \]

(2)

Note that \( 0 \leq D(\rho) \leq 1 \) for all ρ acting on A ⊗ B. We now summarize our results regarding D(ρ).

Summary of results and organization of paper

(A) Our first result is a closed-form expression for \( D(\rho) \) for (2 × N)-dimensional systems (Sec. III). This reveals that for (2 × N)-dimensional ρ, \( D(\rho) \) coincides with the
geometric discord of ρ. It also allows us to prove that, like the Fu distance [27,28], if \( D(\rho) > 1/\sqrt{2} \) for two-qubit ρ, then ρ violates the Clauser-Horne-Shimony-Holt (CHSH) inequality [29]. The Fu distance, defined as the maximization of Eqn. (1) over all \( |U_A, \rho_B(\rho)| = 0 \), was defined in Ref. [27] and studied further in Refs. [28] and [8] with regards to quantifying entanglement and non-classicality.

(B) We next derive a closed form expression for \( D(\rho) \) for Werner states (Sec. [V]), finding here that \( D(\rho) \) in fact equals the Fu distance of ρ.

(C) Sec. [V] proves that only pure maximally entangled states ρ achieve the maximum value \( D(\rho) = 1 \). This is contrast to the Fu distance, which can attain its maximum value even on non-maximally entangled pure states [28].

(D) In Sec. [VI] we show that \( D(\rho) \) is a faithful non-classicality measure, i.e. it achieves a value of zero if and only if ρ is classically correlated in \( \mathcal{A} \). To prove this, we first derive a new characterization of states with zero quantum discord based on the correlation matrix of \( \rho \). We then show that the states achieving \( D(\rho) = 0 \) can be characterized in the same way. More generally, by extending our scheme to allow the eigenvalues of \( U_A \) to have multiplicity at most \( k \), we prove a state is undisturbed under \( U_A \) if and only if there exists a projective measurement on \( \mathcal{A} \) of rank at most \( k \) acting invariantly on the state (Thm. [10]). This reproduces in a simple fashion a result of Ref. [30] regarding entanglement quantification in the pure state setting. Based on this equivalence between disturbance under local unitary operations and local projective measurements, we propose a generalized definition of the quantum discord at the end of Sec. [VI]. In terms of previous work, we note that unlike \( D(\rho) \), the Fu distance is not a faithful non-classicality measure [8]. Alternative characterizations of zero discord states have been given in [21, 25, 31].

(E) Finally, we characterize the set of maximally non-classical, yet separable, \( (2 \times N) \)-dimensional ρ of rank at most two, according to \( D(\rho) \) (and hence according to the geometric discord) (Sec. [VII]). Maximally non-classical separable two-qubit states have previously been studied, for example, in [32,33]. For example, the set of such states found in Ref. [32] with respect to the relative entropy of quantumness matches our characterization for \( D(\rho) \); we remark, however, that our analysis for \( D(\rho) \) in this regard is more general than in [32] as it is based on a less restrictive ansatz.

Sec. [III] begins with necessary definitions and useful lemmas. We conclude in Sec. [VIII] We remark that subsequent to the conception of our scheme, the present author learned that there has also been an excellent line of work studying (the square of) Eqn. (2) in another setting — that of pure state entanglement. In Ref. [34], it was found that in \( (2 \times N) \) and \( (3 \times N) \) systems, \( D(\psi(\psi))^2 \) coincides with the linear entropy of entanglement. Ref. [30] then showed that for arbitrary bipartite pure states, \( D(\psi(\psi))^2 \) is a faithful entanglement monotone, and derived upper and lower bounds in terms of the linear entropy of entanglement.

II. PRELIMINARIES

We begin by setting our notation, followed by relevant definitions and useful lemmas. Throughout this paper, we use \( \mathcal{A} \) and \( \mathcal{B} \) to denote complex Euclidean spaces of dimensions \( M \) and \( N \), respectively. \( \mathcal{D}(\mathcal{A} \otimes \mathcal{B}), \mathcal{H}(\mathcal{A} \otimes \mathcal{B}), \) and \( \mathcal{U}(\mathcal{A} \otimes \mathcal{B}) \) denote the sets of density, Hermitian, and unitary operators taking \( \mathcal{A} \otimes \mathcal{B} \) to itself, respectively. We define \( \rho_A := \text{Tr}_B(\rho) \) and \( \rho_B := \text{Tr}_A(\rho) \), where := indicates a definition. The Frobenius norm of operator \( A \) is \( \| A \|_F = \text{Tr}(\sqrt{A A^T}) \), and the anti-commutator of \( A \) and \( B \) is \( \{ A, B \} = AB + BA \). The notation \( \text{diag}(\mathbf{v}) \) for complex vector \( \mathbf{v} \) denotes a diagonal matrix with \( \mathbf{v} \) as its diagonal entry, and \( \text{span}(\{ \mathbf{v}_i \}) \) denotes the span of the set of vectors \( \{ \mathbf{v}_i \} \). The minimum (maximum) eigenvalue of Hermitian operator \( A \) is denoted \( \lambda_{\min}(A) \) (\( \lambda_{\max}(A) \)), and its \( i \)-th largest eigenvalue is \( \lambda_i(A) \). Finally, \( \mathbb{N} \) is the set of natural numbers.

Moving to definitions, in this paper we often decompose \( \rho \in \mathcal{D}(\mathcal{A} \otimes \mathcal{B}) \) in terms of a Hermitian basis for \( \mathcal{H}(\mathcal{A} \otimes \mathcal{B}) \) (sometimes known as the Fano form [35]):

\[
\rho = \frac{1}{MN} \left( I^A \otimes I^B + \mathbf{r}^A \cdot \sigma^A \otimes I^B + I^A \otimes \mathbf{r}^B \cdot \sigma^B + \sum_{i=1}^{M^2-1} \sum_{j=1}^{N^2-1} T_{ij} \sigma_i^A \otimes \sigma_j^B \right). \quad (3)
\]

Here, \( \sigma^A \) is a \( (M^2-1) \)-component vector of traceless orthogonal Hermitian basis elements \( \sigma_i^A \) satisfying \( \text{Tr}(\sigma_i^A \sigma_j^A) = 2\delta_{ij}, \mathbf{r}^A \in \mathbb{R}^{M^2-1} \) is the Bloch vector for subsystem \( A \) with \( \mathbf{r}_i^A = \frac{2}{N^2-1} \text{Tr}(\rho_A \sigma_i^A) \), and \( T \in \mathbb{R}^{(M^2-1) \times (N^2-1)} \) is the correlation matrix with entries \( T_{ij} = \frac{MN}{2} \text{Tr}(\sigma_i^A \otimes \sigma_j^B) \). For \( M = 2 \), \( \mathbf{r}_A \) satisfies \( 0 \leq \| \mathbf{r}_A \|_2 \leq 1 \) if and only if \( \rho_A \) is pure. The definitions for subsystem \( B \) are analogous. We now give a useful specific construction for the basis elements \( \sigma_i^A \) [36]. Define \( \{ \sigma_i \}_{i=1}^M = \{ U_{pq}, V_{pq}, W_r \} \), such that for \( 1 \leq p < q \leq M \) and \( 1 \leq r \leq M-1 \), and \( \{ |i\rangle \}_{i=1}^M \) some orthonormal basis for \( \mathcal{A} \):

\[
U_{pq} = |p\rangle\langle q| + |q\rangle\langle p| \quad (4)
\]
\[
V_{pq} = -i|p\rangle\langle q| + i|q\rangle\langle p| \quad (5)
\]
\[
W_r = \sqrt{\frac{2}{r(r+1)}} \left( \sum_{k=1}^r |k\rangle\langle k| - kr(r+1)(r+1) \right). \quad (6)
\]

Note that when \( M = 2 \), this construction yields the Pauli matrices \( \sigma^A = (X,Y,Z) \).
Regarding $D(\rho)$, defining $\rho_f := (U_A \otimes I_B)\rho(U_A^\dagger \otimes I_B)$, we often use the fact that Eqn. (2) can be rewritten as:

$$D(\rho) = \min_{U_A \in \text{RU}(A)} \sqrt{\text{Tr}(\rho^2) - \text{Tr}(\rho \rho_f)}. \quad (7)$$

Finally, we show a simple but important lemma.

**Lemma 1.** $D(\rho)$ is invariant under local unitary operations.

**Proof.** Let $\rho' := (V_A \otimes V_B)\rho(V_A \otimes V_B)^\dagger$ for unitaries $V_A, V_B$. Then in Eqn. (7), $\text{Tr}(\rho'^2) = \text{Tr}(\rho^2)$, and $\text{Tr}(\rho' \rho'_f)$ becomes

$$\text{Tr}(\rho(V_A^\dagger U_A V_A \otimes I_B)\rho(V_A^\dagger U_A V_A \otimes I_B))$$

Observe, however, that $V_A U_A V_A^\dagger$ is still an RU unitary, since we have simply changed basis. Hence, $D(\rho', U_A) = D(\rho, V_A^\dagger U_A V_A)$, and since we are minimizing over all $U_A \in \text{RU}(A)$, the claim follows.

**III. $(2 \times N)$-DIMENSIONAL STATES**

In this section, we study $D(\rho)$ for $\rho \in D(\mathbb{C}^2 \otimes \mathbb{C}^N)$, obtaining among other results a closed expression for $D(\rho)$. To begin, note that any $U_A \in \text{RU}(A)$ must have the form

$$U_A := |c\rangle \langle c| - |d\rangle \langle d| = 2|c\rangle \langle c| - I_2, \quad (8)$$

up to an irrelevant global phase which disappears upon application of $U_A$ to our system, and for some orthonormal basis $\{|c\rangle, |d\rangle\}$ for $\mathbb{C}^2$. Then, $D(\rho, U_A)$ can be rewritten as

$$2\sqrt{\text{Tr}([\rho^2|c\rangle \langle c| \otimes I - \rho(|c\rangle \langle c| \otimes I]\rho(|c\rangle \langle c| \otimes I])}. \quad (9)$$

We begin with a simple upper bound on $D(\rho)$.

**Theorem 1.** For any $\rho \in D(\mathbb{C}^2 \otimes \mathbb{C}^N)$, one has

$$D(\rho) \leq 2\sqrt{\lambda_{\min}(\text{Tr}_{BG}(\rho^2))}.$$ 

**Proof.** Starting with Eqn. (9), by noting that $\text{Tr}[\rho(|c\rangle \langle c| \otimes I)\rho(|c\rangle \langle c| \otimes I)] \geq 0$ and using the fact that $\text{Tr}(\rho(C_A \otimes I_B)) = \text{Tr}(\rho A C_A)$, we have that $D(\rho)$ is at most

$$\min_{|c\rangle \in \mathbb{C}^2} 2\sqrt{\text{Tr}([\rho^2|c\rangle \langle c| \otimes I - \rho(|c\rangle \langle c| \otimes I]\rho(|c\rangle \langle c| \otimes I])} = 2\sqrt{\lambda_{\min}(\text{Tr}_{BG}(\rho^2))}. \quad \square$$

Thm. 1 implies that for pure product $|\psi\rangle \in \mathbb{C}^2 \otimes \mathbb{C}^N$, $D(|\psi\rangle \langle \psi|) = 0$, in agreement with the results in Ref. [14]. By next exploiting the structure of $\rho$ further, we obtain a closed form expression for $D(\rho)$.

**Theorem 2.** For any $\rho \in D(\mathbb{C}^2 \otimes \mathbb{C}^N)$, define $G := r^A(r^A)^T + \frac{2}{N} TT^T$. Then, $D(\rho)$ equals

$$\frac{1}{\sqrt{N}}\sqrt{\text{Tr}(G) - \lambda_{\max}(G)} = \frac{1}{\sqrt{N}}\sqrt{\lambda_2(G) + \lambda_3(G)}. \quad (10)$$

**Proof.** Define $P := \langle c|c\rangle$. Then, beginning with Eqn. (9), by rewriting $\rho$ using Eqn. (3) and applying the fact that the basis elements $\sigma_i$ are traceless, we obtain that $\text{Tr}(\rho^2 P \otimes I - \rho P \otimes I P \otimes I)$ equals

$$\frac{1}{4N}\text{Tr}(A_1 - A_2 + A_3 - A_4),$$

where

$$A_1 := \left(\sum_i r_i^A \sigma_i^A\right)^2 P$$

$$A_2 := \left(\sum_i r_i^A \sigma_i^A P\right)^2$$

$$A_3 := \frac{1}{N}\left(\sum_{ij} T_{ij} \sigma_i^A \otimes \sigma_j^B\right)^2 (P \otimes I)$$

$$A_4 := \frac{1}{N}\left(\sum_{ij} T_{ij} \sigma_i^A \otimes \sigma_j^B\right)\left(\sum_{ij} T_{ij} P \sigma_i^A P \otimes \sigma_j^B\right).$$

Using the facts that $(\sigma_i^A)^2 = I$, $\{\sigma_i^A, \sigma_j^A\} = 0$ for $i \neq j$, $\text{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$, and $\text{Tr}(P) = 1$, we thus have

$$\text{Tr}(A_1) = \|r^A\|^2_2, \quad \text{Tr}(A_3) = \frac{2}{N}\sum_{ij} T_{ij}^2$$

$$\text{Tr}(A_2) = \sum_{ij} r_i^A r_j^A \langle c|\sigma_i^A |c\rangle \langle c|\sigma_j^A |c\rangle$$

$$\text{Tr}(A_4) = \frac{2}{N}\sum_{ij} \left(\sum_k T_{ik} T_{jk}\right) \langle c|\sigma_i^A |c\rangle \langle c|\sigma_j^A |c\rangle.$$ 

Now, $\langle c|\sigma_i^A |c\rangle$ can be thought of as the $i$th component of the Bloch vector $v \in \mathbb{R}^3$ of pure state $|c\rangle$ with $\|v\|_2 = 1$, implying

$$\text{Tr}(A_2 + A_4) = v^T \left[r^A(r^A)^T + \frac{2}{N} TT^T\right] v.$$ 

Plugging these values into Eqn. (9), we conclude $D(\rho)$ equals

$$\min_{\|v\|_2 = 1} \frac{1}{\sqrt{N}}\sqrt{\|r^A\|^2_2 + \frac{2}{N}\sum_{ij} T_{ij}^2 - \text{Tr}(A_2 + A_4)}.$$

The claim now follows since for any asymmetric $A \in \mathbb{R}^{n \times n}$, $\max_{v \in \mathbb{R}^n} v^T Av = \lambda_{\max}(A). \quad \square$

The expression for $D(\rho)$ in Thm. 2 matches that for the geometric discord $[21, 37]$. Specifically, defining the latter as $\delta_\rho(\rho) = \min_{\sigma \in \Omega} \sqrt{\|\rho - \sigma\|_F}$, where $\Omega$ is the set of zero-discord states, we have for $(2 \times N)$-dimensional $\rho$ that $D(\rho) = \delta_\rho(\rho)$. (Note: The original definition of Ref. [21] was more precisely $\delta_\rho(\rho) = \min_{\sigma \in \Omega} \|\rho - \sigma\|_F^2$.) We now discuss consequences of Thm. 2 beginning with a lower bound which proves useful later.
Corollary 3. For $\rho \in D(\mathbb{C}^2 \otimes \mathbb{C}^N)$, we have
\[
D(\rho) \geq \frac{\sqrt{2}}{N} \sqrt{\lambda_2(TT^T) + \lambda_3(TT^T)}.
\]
This holds with equality if $r^A = 0$, i.e. $\rho_A = \frac{I}{2}$.

Proof. The first claim follows from the fact that:
\[
\lambda_{\max} \left( r^A(r^A)^T + \frac{2}{N} TT^T \right) \leq \|r^A\|_2^2 + \frac{2}{N} \lambda_{\max} (TT^T).
\]
The second claim follows by substitution into Eqn. (10).

For example, for maximally entangled $|\psi\rangle = (|00\rangle + |11\rangle)/\sqrt{2}$, for which $r^B = 0$ and $T = \text{diag}(1,1,1)$, Cor. 3 yields $D(|\psi\rangle\langle\psi|) = 1$, as desired. We also remark that Eqn. (10) can further be simplified for two-qubit states, since by Ref. [32, 39], one can assume without loss of generality that $T$ is diagonal. This relies on the facts that (1) applying local unitary $V_1 \otimes V_2$ to $\rho$ has the effect of mapping $T \mapsto O_1TO_1^T$, $r^A \mapsto r^A$, and $r^B \mapsto r^B$ for any orthogonal rotation matrices $O_1$ and $O_2$, and (2) $D(\rho)$ is invariant under local unitaries by Lem. 1.

Using Cor. 3 we next obtain a connection to the CHSH inequality for two-qubit $\rho$. Defining $M(\rho) := \lambda_1(TT^T) + \lambda_2(TT^T)$, it is known that $\rho$ violates the CHSH inequality if and only if $M(\rho) > 1$ [40]. We thus have:

Corollary 4. For $\rho \in D(\mathbb{C}^2 \otimes \mathbb{C}^2)$, if $D(\rho) > 1/\sqrt{2}$, then $M(\rho) > 1$. The converse does not hold.

Proof. The first is immediate from Cor. 3 and the fact that $TT^T$ and $T^TT$ are cospectral (Thm. 1.3.20 of [41]). The converse proceeds similarly to Thm. 7 of Ref. [28] — namely, let $|\psi\rangle = a|00\rangle + b|11\rangle$ for real $a, b \geq 0$ and $a^2 + b^2 = 1$. Then, for density operator $|\psi\rangle\langle\psi|$, we have $r^B = (0, 0, a^2 - b^2)$ and $T = \text{diag}(2ab, -2ab, 1)$, implying $M(|\psi\rangle\langle\psi|) > 1$ for $a, b \neq 0$. In comparison, $D(|\psi\rangle\langle\psi|) = 2ab \leq 1/\sqrt{2}$ when $a \leq \sqrt{\frac{1}{2} - \frac{1}{2\sqrt{2}}}$ or $a \geq \sqrt{\frac{1}{2} + \frac{1}{2\sqrt{2}}}$.

Interestingly, the exact same relationship as that in Cor. 3 was found between the Fu distance and the CHSH inequality in Ref. [28].

IV. WERNER STATES

We now derive a closed formula for $D(\rho)$ for Werner states $\rho \in D(\mathbb{C}^d \otimes \mathbb{C}^d)$ where $d \geq 2$, which are defined as [42]
\[
\rho := \frac{2p}{d^2 + d} P_a + \frac{2(1-p)}{d^2 - d} P_a,
\]
for $P_a := (I + P)/2$ and $P_a := (I - P)/2$ the projectors onto the symmetric and anti-symmetric subspaces, respectively. $P := \sum_{i,j=1}^d |i\rangle\langle j| \otimes |j\rangle\langle i|$ the SWAP operator, and $0 \leq p \leq 1$. Werner states are invariant under $U \otimes U$ for any unitary $U$, and are entangled if and only if $p < 1/2$.

Theorem 5. Let $\rho \in D(\mathbb{C}^d \otimes \mathbb{C}^d)$ be a Werner state. Then
\[
D(\rho) = \frac{|2pd - d - 1|}{d^2 - 1}.
\]

Proof. As done in Thm. 3 of Ref. [28], we first rewrite Eqn. (7) using the facts that $\text{Tr}(P) = d$, $\text{Tr}(P^2) = d^2$, and $\beta := \text{Tr}(P(U_A \otimes I)P(U_A \otimes I)^\dagger) = \text{Tr}(U_A)\text{Tr}(U_A^\dagger)$ to obtain that for any $U_A \in U(A)$,
\[
D(\rho, U_A) = \frac{\sqrt{(2pd - d - 1)^2(d^2 - \beta)}}{d^2 - 1}.
\]
Since $\text{Tr}(U_A) = 0$ for any $U_A \in RU(A)$, we have $\beta = 0$ and the claim follows.

Again, we find that this coincides exactly with the expression for the Fu distance for Werner states [28]. Further, Thm. 5 implies that the quantum discord of Werner state $\rho$ is zero if and only if $p = (d + 1)/2d$. This matches the results of Chitambar [43], who develops the following closed formula for the discord $\delta(\rho)$ of Werner states:
\[
\delta(\rho) = \log(d + 1) + (1 - p)\log\frac{1 - p}{d - 1} + p\log\frac{p}{d + 1} - \frac{2p}{d + 1}\log p - \left(1 - \frac{2p}{d + 1}\right)\log\frac{d + 1 - 2p}{2(d - 1)}.
\]
In Sec. VII we show that this is no coincidence — it turns out that $D(\rho) = 0$ if and only if the discord of $\rho$ is zero for any $p$.

V. PURE STATES OF ARBITRARY DIMENSION

We now show that only pure maximally entangled states $\rho$ achieve $D(\rho) = 1$. As mentioned in Sec. IV, this is in contrast to the Fu distance [27, 28], whose maximal value is attained even for certain non-maximally entangled $|\psi\rangle$. We remark that Thm. 6 below also follows from a more general non-trivial result that $D(|\psi\rangle\langle\psi|)^2$ is tightly upper bounded by the linear entropy of entanglement of pure state $|\psi\rangle$ [30]. However, our proof of Thm. 6 is much simpler and requires only elementary linear algebra.

To begin, assume without loss of generality that $M \leq N$, and let $|\psi\rangle \in A \otimes B$ be a pure quantum state with Schmidt decomposition $|\psi\rangle = \sum_{k=1}^M \alpha_k |a_k\rangle \otimes |b_k\rangle$, i.e. $\sum_k \alpha_k^2 = 1$ for $\alpha_k \in \mathbb{R}$ and $\{|a_k\rangle\}$ and $\{|b_k\rangle\}$ the Schmidt bases for $A$ and $B$, respectively.

Theorem 6. Let $|\psi\rangle \in A \otimes B$ with Schmidt decomposition as above. Then $D(|\psi\rangle\langle\psi|) = 1$ if and only if $\alpha_k = \frac{1}{\sqrt{M}}$ for all $1 \leq k \leq M$ (i.e. $|\psi\rangle$ is maximally entangled).

Proof. We begin by rewriting Eqn. (7) as
\[
D(|\psi\rangle\langle\psi|) = \min_{U_A \in RU(A)} \sqrt{1 - \sum_{k=1}^M \alpha_k^2 |U_A(a_k)|^2}.
\]
If $|\psi\rangle$ is maximally entangled, then $\alpha_k = 1/\sqrt{M}$ for all $1 \leq k \leq M$. Then, since $U_A \in \mathcal{R}(A)$, Eqn. (13) yields

$$D(|\psi\rangle\langle\psi|) = \min_{U_A \in \mathcal{R}(A)} \sqrt{1 - \frac{1}{M^2} |Tr(U_A)|^2} = 1.$$ 

For the converse, assume $D(|\psi\rangle\langle\psi|) = 1$. Then, by Eqn. (13), we must have that for all $U_A \in \mathcal{R}(A)$,

$$\sum_{k=1}^{M} \alpha_k^2 \langle a_k|U_A|a_k\rangle = 0. \quad (14)$$

Thus, choosing $U_A$ as diagonal in basis $\{|a_k\rangle\}$, Eqn. (14) equivalently says that $w^T \pi v = 0$ for all permutations $\pi \in S_M$, where $w_k := \alpha_k^2$ and $v_k := e^{2\pi ki/M}$. This can only hold, however, if all entries of $w$ are the same, i.e. $\alpha_k = 1/\sqrt{M}$ for all $1 \leq k \leq M$, as desired. \hfill \Box

**Corollary 7.** A quantum state $\rho \in \mathcal{D}(A \otimes B)$ achieves $D(\rho) = 1$ if and only if $\rho$ is pure and maximally entangled.

**Proof.** Immediate from Thm. 6 and the $\text{Tr}(\rho^2)$ in Eqn. (7). \hfill \Box

## VI. RELATIONSHIP TO QUANTUM DISCORD

We now show that for arbitrary $\rho \in \mathcal{D}(A \otimes B)$, $D(\rho)$ is zero if and only if the quantum discord of $\rho$ is zero. The discord is defined as follows [25]:

$$\delta(\rho) := S(A) - S(A,B) + \min_{\{\Pi_A^i\}} S(B|\{\Pi_A^i\}), \quad (15)$$

where $\{\Pi_A^i\}$ corresponds to a complete measurement on subsystem $B$ consisting of rank 1 projectors, $S(B) = -\text{Tr}(\rho_B \log(\rho_B))$ is the von Neumann entropy of $\rho_B$, similarly $S(A,B) = S(\rho)$, and

$$S(B|\{\Pi_A^i\}) = \sum_j p_j S\left(\frac{1}{p_j} \Pi_A^j \otimes I^B \rho \Pi_A^j \otimes I^B\right), \quad (16)$$

where $p_j = \text{Tr}(\Pi_A^j \otimes I^B \rho)$. Here, the main fact we leverage about the discord is the following.

**Theorem 8** (Ollivier and Zurek [25]). For $\rho \in \mathcal{D}(A \otimes B)$, $\delta(\rho) = 0$ if and only if

$$\rho = \sum_j \Pi_A^j \otimes I^B \rho \Pi_A^j \otimes I^B, \quad (17)$$

for some complete set of rank 1 projectors $\{\Pi_A^i\}$.

We now prove the main result of this section. The first part of the proof involves a new characterization of the set of zero discord quantum states $\rho$ in terms of the basis elements $\sigma^A_i$ from the Fano form of $\rho$. Key to this characterization is the absence of non-diagonal $\sigma^A_i$ in the expansion of $\rho$. In the proofs below, we assume the basis elements $\sigma^A_i$ for $A$ come from the set $\{I, U_{pq}, V_{pq}, W_r\}_{p,q,r}^A$ from Sec. [I](analogously for $B$).

**Theorem 9.** Let $\rho \in \mathcal{D}(A \otimes B)$. Then $\delta(\rho) = 0$ if and only if there exists a local unitary $V^A$ such that

$$\text{Tr}\left((V^A \otimes I^B) \rho (V^A \otimes I^B)^\dagger (\sigma^A_i \otimes \sigma^B_j)\right) = 0$$

for all $\sigma^A_i \in \{U_{pq}, V_{pq}\}^A$ and all $\sigma^B_j \in \{I, U_{pq}, V_{pq}, W_r\}^B$. The same characterization holds for $D(\rho) = 0$.

**Proof.** We prove the equivalent statement that $\delta(\rho) = 0$ if and only if there exists an orthonormal basis $\{|k\rangle\}$ for $A$ such that, for basis elements $\sigma^A_i$ constructed with respect to $\{|k\rangle\}$, we have $\text{Tr}(\rho(\sigma^A_i \otimes \sigma^B_j)) = 0$ for all $\sigma^A_i \in \{U_{pq}, V_{pq}\}$ (and similarly for $D(\rho) = 0$).

Suppose $\delta(\rho) = 0$. Then by Thm. 8 there exists a complete set of rank 1 projectors $\{\Pi_A^i\}$ such that Eqn. (17) holds. Let $\{|k\rangle\}$ be the basis onto which $\{\Pi_A^i\}$ projects, and define $\Phi(C) := \sum_i \Pi_A^i U_A C U_A^\dagger$. By constructing the basis elements $\sigma^A_i$ in Eqn. (3) using $\{|k\rangle\}$, we thus have

$$\rho = \frac{1}{MN} \left[ I^A \otimes I^B + I^A \otimes \gamma^B \cdot I^B + \sum_{i=1}^{M-1} \Phi(\sigma^A_i) \otimes \left( v_i^A I^B + \sum_{j=1}^{N-1} T_{ij} \sigma^B_j \right) \right]. \quad (18)$$

Now, for all $\sigma^A_i \in \{W_r\}$, we clearly have $\Phi(\sigma^A_i) = \sigma^A_i$. For $\sigma^A_i \in \{U_{pq}, V_{pq}\}$, however, $\Phi(\sigma^A_i) = 0$. Thus, in order for Eqn. (17) to hold, we must have $T_{ij} = 0$ for all basis elements $\sigma^A_i \in \{U_{pq}, V_{pq}\}$, which by definition means $\text{Tr}(\rho(\sigma^A_i \otimes \sigma^B_j)) = 0$ for all $\sigma^A_i \in \{U_{pq}, V_{pq}\}^A$, as desired. To show that this implies $D(\rho) = 0$, construct $U_A \in \mathcal{R}(A)$ as diagonal in basis $\{|k\rangle\}$ and define $\Phi(C) := U_A C U_A^\dagger$. Then since in Eqn. (13), we have $\Phi(\sigma^A_i) = \sigma^A_i$ for any $\sigma^A_i \in \{I, W_r\}$, the claim follows.

To show the converse, assume $D(\rho, U_A) = 0$ for some $U_A \in \mathcal{R}(A)$. Then, construct the basis elements $\sigma^A_i$ with respect to a diagonalizing basis $\{|k\rangle\}$ for $A$ and define $\Phi(C) := U_A C U_A^\dagger$. It follows that for any $p$ and $q$,

$$\Phi(U_{pq}) = e^{i(\theta_p - \theta_q)} |p\rangle\langle q| + e^{-i(\theta_p - \theta_q)} |q\rangle\langle p|, \quad (19)$$

$$\Phi(V_{pq}) = -ie^{i(\theta_p - \theta_q)} |p\rangle\langle q| + ie^{-i(\theta_p - \theta_q)} |q\rangle\langle p|. \quad (20)$$

Consider now an arbitrary term $(c_u \sigma^A_u + c_v \sigma^A_v) \otimes \sigma^B_j$ from the Fano form of $\rho$ where $\sigma^A_u = U_{pq}$ and $\sigma^A_v = V_{pq}$ for some choice of $p$ and $q$. Since Eqns. (19) and (20) imply that $U_A$ can only map $U_{pq}$ to $V_{pq}$ and vice versa, it follows that in order for $D(\rho, U_A) = 0$ to hold, we must have $\Phi(c_u \sigma^A_u + c_v \sigma^A_v) = c_u \sigma^A_u + c_v \sigma^A_v$. This leads to the system of equations

$$c_u - ic_v = e^{i(\theta_p - \theta_q)} (c_u - ic_v)$$

$$c_u + ic_v = e^{-i(\theta_p - \theta_q)} (c_u + ic_v).$$

We conclude that if either $c_u \neq 0$ or $c_v \neq 0$, it must be that $\theta_p = \theta_q$ in order for $D(\rho) = 0$ to hold. However, since all
Theorem 10. Let $\rho \in D(A \otimes B)$ and $v \in \mathbb{N}^M$ such that $\sum_{j=1}^M v_j = M$. Then, there exists a complete projective measurement $\{\Pi_j\}_v$ such that

$$\rho = \sum_j \Pi_j^A \otimes I^B \rho \Pi_j^A \otimes I^B$$

if and only if there exists a $U^A \in \mathcal{U}(A)$ with $D(\rho, U^A) = 0$.

Proof. The proof follows that of Thm. 9 so we outline the differences. Here, $U^A$ and $\{\Pi_j\}_v$ will be related through the correspondence outlined above, and the basis elements $\sigma^A$ are constructed with respect to a diagonalizing basis $\{|k\rangle\}$ for $U^A$ (which by definition also diagonalizes each $\Pi_j^A \in \{\Pi_j\}_v$). For simplicity, we discuss the case of $v = (M - 2, 1, 0, \ldots, 0)$; all other cases proceed analogously.

Going in the forward direction, suppose $\Pi_j^A \in \{\Pi_j\}_v$ projects onto $S_{pq} := \text{span}(|p\rangle, |q\rangle)$. Then, in Eqn. (18), $\Phi(\sigma^A_j) = \sigma^A_j$ for $\sigma^A_j = U^A_{pq}$ and $\sigma^A_j = V^A_{pq}$. In other words, we now have $v_i^A \neq 0$ and $T_i \neq 0$ (however, note we still have $T_{m \neq i,j} = 0$). Since $U^A_{pq}$ has a degenerate eigenvalue on $S_{pq}$, however, we have by Eqs. (19) and (20) that $U^A_{pq}$ acts invariantly on $\sigma^A_j$ as well (since $\theta_p = \theta_j$). The converse is similar; namely, suppose $U^A_{pq}$ has a degenerate eigenvalue on $S_{pq}$. Then the projector onto the corresponding two-dimensional eigenspace $\Pi_j^A \in \{\Pi_j\}_v$ is $\Pi_j^A = |p\rangle\langle p| + |q\rangle\langle q|$. It thus follows by the same argument as above that both $U^A_{pq}$ and $\Pi_j^A$ act invariantly on $U^A_{pq}$ and $V^A_{pq}$.

From this general theorem, we can re-derive as a simple corollary the pure state result of Ref. [60] mentioned earlier, which we rephrase in our terminology as follows.

Corollary 11. Let $|\psi\rangle = \sum_{i=1}^M \alpha_i |\psi^A_i\rangle |\psi^B_i\rangle$ be the Schmidt decomposition of $|\psi\rangle \in A \otimes B$. Then, there exists $U^A_{pq} \in \mathcal{U}(A)$ with $v_k \geq 1$ (i.e. $U^A_{pq}$ has an eigenvalue of multiplicity $k$), $v_{k+1} = 0$ (all eigenvalues of $U^A_{pq}$ have multiplicity at most $k$), and $D(|\psi\rangle\langle \psi|, U^A_{pq}) = 0$ if and only if $k \geq r$.

Proof. Suppose $k \geq r$. Then, by defining $\{\Pi_j\}_v$ such that $v_k \geq 1$ and $v_{k+1} = 0$, one can choose a $\{\Pi_j\}_v$ such that Eqn. (21) holds for $\rho = |\psi\rangle\langle \psi|$. Conversely, consider any $\{\Pi_j\}_v$ such that Eqn. (21) holds. By Thm. 10 this implies that there exists a $U^A_{pq}$ with $v_k \geq 1$ and $v_{k+1} = 0$ achieving $D(|\psi\rangle\langle \psi|, U^A_{pq}) = 0$. Conversely, if $k < r$, then clearly no such $\{\Pi_j\}_v$ exists such that Eqn. (21) holds exists. By Thm. 10 this implies that no $U^A_{pq}$ with an eigenvalue of multiplicity at most $k$ and $D(|\psi\rangle\langle \psi|, U^A_{pq}) = 0$ exists, as desired.

We close this section with two final comments. First, given Thm. 9 one might ask whether a stronger relationship between $D(\rho)$ and $\delta(\rho)$ holds. For example, could it be that $D(\rho) \geq \delta(\rho)$ for all $\rho$? This simplest type of relationship is ruled out easily via Thm. 5 and Eqn. (12), since for $d = 2$ and $p = 2/3$, $D(\rho) = 1/9 \geq \delta(\rho) \approx 0.01614$, while for $d = 50$ and $p = 2/3$, $D(\rho) \approx 0.00627 \geq \delta(\rho) \approx 0.07111$.

Second, note that Thm. 10 reduces to Thm. 9 if we choose $v = (M, 0, \ldots, 0)$. This suggests defining a generalized quantum discord, denoted $\delta_v(\rho)$, which is analogous to $\delta(\rho)$, except that now we use the class of measurements $\{\Pi_j^A\}_v$ in Eqn. (15). For example, $\delta_{(M,0)}(\rho) = \delta(\rho)$. We hope the study of $\delta_v(\rho)$ would prove fruitful in its own right.
VII. MAXIMALLY NON-CLASSICAL SEPARABLE STATES

In this section, we characterize the set of maximally non-classical, yet separable, \((2 \times N)\)-dimensional states of rank at most 2, as quantified by \(D(\rho)\). To do so, consider separable state

\[
\rho = \sum_{i=1}^{n} p_i \ket{a_i} \bra{a_i} \otimes \ket{b_i} \bra{b_i},
\]

where \(\sum_i p_i = 1\), \(\ket{a_i} \in \mathbb{C}^2\), \(\ket{b_i} \in \mathbb{C}^N\). Via simple algebraic manipulation, one then finds that \(D(\rho, U_A)\) for any given \(U_A \in U(A)\) is given by

\[
\sqrt{\sum_{i,j} p_i p_j |\langle b_i | b_j \rangle|^2 (|\langle a_i | a_j \rangle|^2 - |\langle a_i | U_A(a_j) \rangle|^2)}. \tag{23}
\]

We begin by proving a simple but useful upper bound on \(D(\rho)\) which depends solely on \(n\).

Lemma 2. Let \(\rho\) be a separable state as given by Eqn. 22. Then \(D(\rho) \leq 1 - \max_i p_i \leq 1 - \frac{1}{n}\).

Proof. Assume WLOG that \(\max_i p_i = p_1\). Then \(1/n \leq p_1 \leq 1\). Choose any \(U_A \in U(A)\) such that \(\ket{a_1}\) is an eigenvector of \(U_A\). Then any term in the double sum of Eqn. (23) in which \(\ket{a_1}\) appears vanishes. We can hence loosely upper bound the value of Eqn. (23) by \(\sqrt{\sum_{i \neq j \neq 1} p_i p_j} = 1 - p_1\). Recalling that \(p_1 \geq 1/n\) yields the desired bound.

When \(n = 2\), i.e. when \(\rho\) is rank at most two, observe from Lem. 2 that \(D(\rho) \leq 1/2\), and this is attainable only when \(p_1 = p_2 = 1/2\). We now show that this bound can indeed be saturated, and characterize all states with \(n = 2\) that do so.

Lemma 3. Let \(\rho\) be a separable state as in Eqn. (22) with \(p_1 = p_2 = 1/2\). Then \(D(\rho) = 1/2\) if and only if \(|\langle a_1 | a_2 \rangle| = 1/\sqrt{2}\) and \(|\langle b_1 | b_2 \rangle| = 0\).

Proof. Since by Lem. 1 \(D(\rho)\) is invariant under local unitaries, we can assume without loss of generality that \(\ket{a_1} = \ket{0}\), \(\ket{b_1} = \ket{0}\), \(\ket{a_2} = \cos \frac{\theta}{2} \ket{0} + \sin \frac{\theta}{2} \ket{1}\) and \(\ket{b_2} = \sum_{i=0}^{N-1} \alpha_i \ket{i}\) for \(\beta \in [0, \pi]\) and \(\alpha_i \in \mathbb{R}\) with \(\sum_i \alpha_i^2 = 1\), i.e. we can rotate the local states so as to eliminate relative phases. Further, since \(U_A \in RU(A)\) in Eqn. (23), we can write \(U_A = 2 |u \rangle \langle u | - I\) for some \(|u\rangle = \cos \frac{\theta}{2} \ket{0} + e^{i\phi} \sin \frac{\theta}{2} \ket{1}\), where \(\theta, \phi \in [0, 2\pi]\). Via the latter, we can rewrite Eqn. (23) as:

\[
\frac{1}{2} \sqrt{\sum_{i,j} p_i p_j |\langle b_i | b_j \rangle|^2 (|\langle a_i | a_j \rangle|^2 - |\langle a_i | U_A(a_j) \rangle|^2)}. \tag{24}
\]

Letting \(\Delta\) denote the expression under the square root above, we have by substituting in our expressions for \(\ket{a_1}, \ket{a_2}, \ket{b_1}, \ket{b_2}\), and algebraic manipulation that

\[
\Delta = \alpha_0^2 \left[ 2 \cos \beta \sin^2 \theta - \sin \beta \sin(2\theta) \cos \phi \right] + 1 + \sin^2 \theta - (\cos \beta \cos \theta + \sin \beta \sin \theta \cos \phi)^2. \tag{25}
\]

Our goal is to maximize \(\Delta\) with respect to \(\alpha_0\) and \(\beta\) (which define \(\rho\)), and then minimize with respect to \(\theta\) and \(\phi\) (which define \(U_A\)). Observe now that choosing \(\phi = 0\) reduces Eqn. (25) to \(\Delta = 1 - \cos^2 \beta\). Hence, unless \(\beta = \pi/2\) (i.e. \(|\langle a_1 | a_2 \rangle| = 1/\sqrt{2}\)), we can always achieve \(D(\rho) < 1/2\). Thus, set \(\beta = \pi/2\). Consider next \(\phi = 0\), and leave \(\theta\) unassigned. Then, Eqn. (25) reduces to \(\Delta = 1 - \alpha_0^2 \sin(2\theta)\), from which it is clear that unless \(\alpha_0 = 0\) (i.e. \(|b_1 | b_2\rangle = 0\), we can always achieve \(D(\rho) < 1/2\). Plugging these values of \(\alpha_0\) and \(\beta\) into Eqn. (25), we have \(\Delta = 1 + \sin^2 \theta \sin^2 \phi\), from which the claim follows.

For two-qubit \(\rho\), we thus have that with respect to \(D(\rho)\) and the geometric discord, the maximally non-classical two qubit states of rank at most two are, up to local unitaries,

\[
\frac{1}{2} |0\rangle \langle 0 | \otimes |0\rangle \langle 0 | + \frac{1}{2} |+\rangle \langle + | \otimes |1\rangle \langle 1 |,
\]

where \(|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}\). As mentioned earlier, this matches known results with respect to the relative entropy of quantuness [32]. However, the latter analysis is not as general as it begins by with the assumption that \(|b_1 | b_2\rangle = 0\), whereas we allow arbitrary \(|b_1 | b_2\rangle\). It would be interesting to know whether this analysis can be extended to arbitrary rank two-qubit states.

VIII. CONCLUSION

We have shown that local unitary operations can indeed form the basis of a faithful non-classicality measure \(D(\rho)\) with desirable properties such as: Closed-form expressions for \((2 \times N)\)-dimensional systems (which coincided with the expression for the geometric discord) and Werner states, a maximum value being attained only for pure maximally entangled states, and faithfulness. We further showed a direct connection between the degeneracy of the spectrum of local unitaries used in our measure and the ability for a state to remain undisturbed under local projective measurements of higher rank. Finally, we gave a characterization of the set of maximally non-classical, yet separable, \((2 \times N)\)-dimensional \(\rho\) of rank at most two (according to \(D(\rho)\)), and hence also according to the geometric discord.

We leave open the following questions. For what other interesting classes of quantum states can a closed form expression for \(D(\rho)\) be found? Can a better intuitive understanding...
of the interplay between the notions of “disturbance under local measurements” and “disturbance under local unitary operations” be obtained in higher dimensions?

We have given an analytical characterization of all maximally non-classical rank-two \((2 \times N)\)-dimensional separable states — we conjecture that higher rank two-qubit states, for example, achieve strictly smaller values of \(D(\rho)\). Can this be proven rigorously and analytically? (We remark that a numerical proof for this conjecture was given in [33] for the geometric discord, for example.) What can the study of the generalized notion of quantum discord we defined in Sec. [VI] \(\delta_v(\rho)\), tell us about non-classical correlations?

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Note: After completion of this paper, the author learned of independent work in preparation on a similar topic, which has been posted [44] since the first version of the present paper appeared.

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