Discriminating strength: a bona fide measure of non-classical correlations

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Received 12 February 2014, revised 8 May 2014
Accepted for publication 9 May 2014
Published 4 July 2014

Abstract
A new measure of non-classical correlations is introduced and characterized. It tests the ability of using a state $\rho$ of a composite system $AB$ as a probe for a quantum illumination task (e.g. see Lloyd 2008 Science \textbf{321} 1463), in which one is asked to remotely discriminate between the two following scenarios: (i) either nothing happens to the probe, or (ii) the subsystem $A$ is transformed via a local unitary $R_A$ whose properties are partially unspecified when producing $\rho$. This new measure can be seen as the discrete version of the recently introduced interferometric power measure (Girolami \textit{et al} 2013 e-print arXiv:1309.1472) and, at least for the case in which $A$ is a qubit, it is shown to coincide (up to an irrelevant scaling factor) with the local quantum uncertainty measure of Girolami, Tufarelli and Adesso (2013 \textit{Phys. Rev. Lett}. \textbf{110} 240402). Analytical expressions are derived which allow us to formally prove that, within the set of separable configurations, the maximum value of our non-classicality measure is achieved over the set of quantum-classical states (i.e. states $\rho$ which admit a statistical unravelling where each element of the associated ensemble is distinguishable via local measures on $B$).

Keywords: quantum correlations, state discrimination, quantum metrology, quantum discord, quantum information
1. Introduction

In recent years strong evidence has been collected in support of the fact that composite quantum systems can exhibit correlations which, while not being accountable for by a purely classical statistical theory, still go beyond the notion of quantum entanglement [1]. In the seminal papers by Henderson and Vedral [2], and Ollivier and Zurek [3], this new form of non-classicality was gauged in terms of a difference of two entropic quantities—specifically the quantum mutual information [4] (which accounts for all correlations in a bipartite system), and the Shannon mutual information [5] extractable by performing a generic local measurement on one of the subsystems. The resulting functional, known as quantum discord [2], enlightens the impossibility of recovering the information contained in a composite quantum system by performing local detections only. It turns out that this intriguing feature of quantum mechanics is not directly related to entanglement [6]. Indeed, even though all entangled states are bound to exhibit a non-zero value of quantum discord, examples of separable (i.e. non-entangled) configurations can be easily found which share the same property—zero value of discord identifies only a tiny (zero-measure) subset of all separable configurations [7]. In spite of the enormous effort spent in characterizing this emerging new aspect of quantum mechanics, a question which is still open is whether and to what extent the new form of quantum correlations identified by quantum discord can be considered as a resource and exploited to give some kind of advantage over purely classical means. Due to the variety of contexts where quantum theory has proved to be a useful tool for developing new technological ideas (such as information theory, thermodynamics, computation and communication), this has given rise to a number of alternative definitions and quantifiers of discord-like correlations, see e.g. [1] and references therein. This proliferation stems also from the difficulty of identifying a measure which is at the same time well defined, easily computable (even for the case of a two-qubit system), and has a clear operative meaning. As a paradigmatic example, let us recall the geometric discord [8] which can be effortlessly computed at the price of increasing under local operations [9]. Some geometric alternatives have been proposed in order to overcome this hindrance. For example one can take the Hilbert–Schmidt distance between the square root of density operators, rather than the density operators themselves [10], or use different distances such as the trace distance [11] and the Bures distance [12]. There are also several non-geometric approaches to quantum correlations, both on a fundamental and on an applied level. Among them, let us briefly recall the measurement-induced disturbance [13] and non-locality [14], which consider the perturbation induced by local von Neumann measurements on non-classically correlated states. On the other hand, the quantum deficit [15] investigates the role of quantum discord in work extraction from a heat bath, while the so-called quantum advantage [16] focuses on quantum discord as the resource allowing quantum communication to be more efficient than classical communication.

Dealing with this complex scenario, here we introduce a new measure of quantum correlations, the discriminating strength (DS), which turns out to be a valid tradeoff between computability and the fulfillment of the criteria that every good discord quantifier should satisfy [17]. Most importantly, it also possesses a clear operative meaning, being directly connected with the quantum illumination procedures introduced in [18–21]. Being the counterpart of the recently introduced interferometric power (IP) for continuous variable estimation theory [22], the DS enlightens the benefit gained by quantum state discrimination protocols when general quantum correlations, not necessarily in the form of entanglement, are employed. Finally, we
provide a formal connection between our new measure and the local quantum uncertainty (LQU) measure introduced in [23] whose operational meaning was not yet completely understood. Specifically we show that LQU is a special case of DS when the state is used as a probe to determine the application of a local unitary which is close to the identity. Furthermore, for qubit–qudit systems one can verify that LQU and DS always coincide up to a proportionality factor. The DS, together with the aforementioned IP and LQU, witness a recent burst of attention to the crucial role played by quantum correlations in the realm of quantum metrology.

The manuscript is organized as follows. In section 2 we introduce a paradigmatic state discrimination scheme and we quantify how well a generic state $\rho$ can perform in the discrimination. In section 3 we show that the same quantifier satisfies all the properties required for a bona fide measure of discord. Moreover we present the connection between our measure and the LQU measure and we provide some simple analytical formulas for some special cases (specifically pure states and qubit–qudits systems). In section 4 we focus on the set of separable states and we determine the maximum value of the DS on this set in the qubit–qudits case. Conclusions are left to section 5.

2. DS

In order to formally introduce our new measure of non-classicality it is useful to recall the quantum Chernov bound (QCB) [24]. This is an inequality which characterizes the asymptotic scaling of the minimum error probability $P_{\text{err},\min}^{(n)}(\rho_0, \rho_1)$ attainable when discriminating among $n$-copies of two density matrices $\rho_0$ and $\rho_1$ [24]. By optimizing with respect to all possible positive-operator valued measures (POVMs) aimed to distinguish between the two possible configurations, and assuming a 50% prior probability of getting $\rho_0 \otimes^n$ or $\rho_1 \otimes^n$ [25], one can write

$$P_{\text{err},\min}^{(n)} := \frac{1}{2} \left( 1 - \| \rho_0 \otimes^n - \rho_1 \otimes^n \|_1 \right),$$

(1)

the optimal detection strategy being the one which discriminates between the negative and non-negative eigenspaces of the operator $\rho_0 \otimes^n - \rho_1 \otimes^n$. For large enough $n$, the dependance of the error probability on the number of copies can be approximated by an exponential decay

$$P_{\text{err},\min}^{(n)}(\rho_0, \rho_1) \simeq e^{-n \xi(\rho_0, \rho_1)} =: Q(\rho_0, \rho_1)^n,$$

(2)

characterized by the decay constant

$$\xi(\rho_0, \rho_1) := - \lim_{n \to \infty} \frac{\ln P_{\text{err},\min}^{(n)}(\rho_0, \rho_1)}{n}.$$

(3)

Accordingly, the larger is $Q(\rho_0, \rho_1)$ the less distinguishable are the states $\rho_0$ and $\rho_1$. The limit in (3) corresponds to the QCB bound [24] and reads

$$e^{-\xi(\rho_0, \rho_1)} = Q(\rho_0, \rho_1) = \min_{0 \leq r \leq 1} \text{Tr} \left[ \rho_0^r \rho_1^{1-r} \right],$$

(4)

which implies

$$0 \leq Q(\rho_0, \rho_1) \leq \text{Tr} \left[ \rho_0^{1/2} \rho_1^{1/2} \right] \leq 1.$$

(5)
Furthermore if at least one of the two quantum states $\rho_0$ or $\rho_1$ is pure, then QCB reduces to the Uhlmann’s fidelity [26], i.e.

$$Q(\rho_0, \rho_1) = \mathcal{F}(\rho_0, \rho_1) := \left( \text{Tr} \left[ \sqrt{\sqrt{\rho_0} \rho_1 \sqrt{\rho_0}} \right] \right)^2 .$$

Let us now consider the following quantum illumination scenario [18–21]. A first party (Alice) prepares $n$ copies of a density matrix $\rho$ of a bipartite system $AB$ composed of a probing component $A$ and a reference component $B$, while a second party (the non-cooperative target Robert) selects an undisclosed unitary transformation $R_A$ from a set $\mathcal{S}$ of allowed transformations, should be applied (locally) on each one of the probes $A$. After this action the subsystems $A$ are returned to Alice and the chosen $R_A$ is revealed to her. By exploiting this information and by performing the most general measure on her systems, she has now to determine which option (i.e. the application of $R_A$ or the non-application of $R_A$) Robert has selected.

![Figure 1. Sketch of the discrimination problem discussed in the text. (1) A first party (say Alice) prepares $n$ copies of a bipartite state $\rho$ of a composite system $AB$ and (2) sends the probing subsystems $A$ to a second party (say Robert) while keeping the reference subsystems $B$ on her laboratory. (3) Robert can now decide whether or not a certain unitary rotation $R_A$, which he has previously selected from a set $\mathcal{S}$ of allowed transformations, should be applied (locally) on each one of the probes $A$. (4) After this action the subsystems $A$ are returned to Alice and the chosen $R_A$ is revealed to her. By exploiting this information and by performing the most general measure on her systems, she has now to determine which option (i.e. the application of $R_A$ or the non-application of $R_A$) Robert has selected.](image-url)
where the maximization is performed over the set $S$ of allowed $R_A$, and where the symbol $A \rightarrow B$ enlightens the different role played by the two subsystems in the problem—an asymmetry which is a common trait of the majority of non-classical correlations measures introduced so far [1].

From equations (4) and (7) it is clear that the higher is $D_{A \rightarrow B} (\rho)$ the better Alice will be able to determine whether a generic element of $S$ has been applied or not to $A$. It is a natural guess to expect that the capability shown by the input state $\rho$ of recording the action of an arbitrary local rotation, should increase with the amount of correlations shared between the probe $A$ (which has been affected by the rotation) and the reference $B$ (which has not). This behavior would be analogous to that displayed by the IP measure discussed in [22], which quantifies the worst-case precision in determining the value of a continuous parameter. Clearly the choice of $S$ plays a fundamental role in our construction: for instance allowing $S$ to coincide with the group $U_A$ of all possible unitary transformations on $A$, including the identity, would give $D_{A \rightarrow B} (\rho) = 0$ for all states $\rho$. To avoid these pathological results we find it convenient to identify $S$ with the special family of $R_A$ parametrized as $R_A^\Lambda = \exp[\Lambda_i H_i^A]$, where $H_i^A$ is a Hamiltonian of assigned non-degenerate spectrum represented by the elements of the diagonal matrix

$$\Lambda := \text{Diag} \{\lambda_1, \lambda_2, ..., \lambda_{d_A}\}.$$  

(8)

with $\lambda_1 > \lambda_2 > ... > \lambda_{d_A}$ ($d_A$ being the dimension of the system $A$) and $\lambda_1 - \lambda_{d_A} < 2\pi$ (a condition the latter of which can always be enforced by properly relabeling the entries of $\Lambda$). Accordingly we have

$$H_A^\Lambda = U_A \Lambda U_A^\dagger,$$  

(9)

$$R_A^\Lambda = U_A \exp[i\Lambda] U_A^\dagger,$$  

(10)

where now $U_A$ spans the whole set $U(d_A)$. For each given choice of $\Lambda$ (8) we thus define the quantity

$$D_{A \rightarrow B} (\rho) := 1 - \max_{\{H_A^\Lambda\}} \left( \rho, e^{iH_A^\Lambda} \rho e^{-iH_A^\Lambda} \right),$$  

(11)

the maximization being performed over the set $\{H_A^\Lambda\}$ of the Hamiltonians of the form (9). This measure of discord can be interpreted as an extension to generic non-classical correlations of the entanglement of response, which quantifies the change induced on the state of a composite quantum system by local unitary transformations [27]. In this respect another measure of discord has been recently introduced, the *discord of response* (DR) [28]. The DR is defined in terms of a maximization, over the set of unitary operators endowed with fully non-degenerate spectrum in the roots of the unity, of the Bures distance between the considered state and its evolution under such unitary transformations. Similarly to the DS, the DR accounts for the degree of distinguishability between an assigned quantum state and its evolution under local unitary operators. However, in the case of the DS introduced in this paper, no further limitations, apart from the non-degeneracy, are imposed on the spectrum of the unitary operators.
In the next section we will show that, for all given choices of the spectrum \( \Lambda \) the functional (11) fulfills all the requirements necessary for attesting it as a proper measure of non-classical correlations [1].

3. Properties

In this section we show that the DS (11) is a bona fide measure of non-classicality. We also clarify the connection between our measure and the LQU measure introduced by Girolami et al in [23]. Finally we provide close analytical expressions that, in some special cases, allow one to avoid going through the cumbersome optimization over the set \( \{ H_A^i \} \) of the Hamiltonians (9).

3.1. DS as a measure of non-classical correlations

**Theorem 1.** \( D_{A\rightarrow B}^\Lambda (\rho) \) satisfies the following properties:

1. it nullifies if and only if \( \rho \) is a classical-quantum (CQ) state (12)
   \[
   \rho = \sum_i p_i \ket{i}_A \bra{i} \otimes \rho_{B}^{(i)},
   \]  
   with \( p_i \) being probabilities, \( \{ \ket{i}_A \} \) being an orthonormal basis of \( A \) and \( \{ \rho_{B}^{(i)} \} \) being a collection of density matrices of \( B \) (these are the only configurations for which it is possible to recover partial information on the system by measuring \( A \), without introducing any perturbation [1]);

2. it is invariant under the action of arbitrary local unitary maps, \( W_A \) and \( V_B \) on \( A \) and \( B \) respectively, i.e.
   \[
   D_{A\rightarrow B}^\Lambda (\rho) = D_{A\rightarrow B}^\Lambda (W_A \otimes V_B \rho W_A^\dagger \otimes V_B^\dagger); \tag{13}
   \]

3. it is non-increasing under any completely positive, trace-preserving [29] map \( \Phi_B \) on \( B \);

4. it is an entanglement monotone when \( \rho \) is pure.

**Proof.**

(1) \( D_{A\rightarrow B}^\Lambda (\rho) = 0 \) iff there exists at least an element of the set (9) such that \( Q \left( \rho, R_A^4 \rho R_A^{4\dagger} \right) = 1 \). The latter condition is satisfied iff \( \rho = R_A^4 \rho R_A^{4\dagger} \). Being \( R_A^4 \) endowed with a non-degenerate spectrum, this is equivalent to stating that \( \rho \) and \( H_A^i \) are diagonal in the same basis \( \{ i \}_A \) of \( \mathcal{H}_A \), and thus \( \rho \) reduces to a CQ state of the form (12).

(2) First note that for every unitary operator \( U \) it holds \( (U \rho U^\dagger)^\dagger = U \rho^\dagger U^\dagger \). Then, due to the cyclic property of the trace, \( V_B^\dagger \) cancels out with \( V_B^\dagger \) in the computation of \( Q \). Finally \( W_A^\dagger H_A^i W_A \) has the same spectrum of \( H_A^i \) so that the maximization domain in (11) remains unchanged along with the maximum value.

(3) This follows from the very definition of the QCB. Indeed, the minimum error probability in (1) is achieved by optimizing over all possible POVM measurements on \( (AB)^{\otimes n} \). Any local map \( \Phi_B \) on \( B \) commutes with the phase transformation determined by \( H_A^i \), and thus can be
reabsorbed in the measurement process. This modified measurement is at most as good as the optimal one, implying that the asymptotic error probability, and hence \( Q \), cannot decrease. This gives \( D_{A\rightarrow B}^{\Lambda} (\Phi_{B} [\rho]) \leq D_{A\rightarrow B}^{\Lambda} (\rho) \).

(4) We will prove that if a pure state \( |\psi\rangle \) is transformed into another pure state \( |\phi\rangle \) by local operations and classical communication (LOCC), then \( D_{A\rightarrow B}^{\Lambda} (|\phi\rangle) \leq D_{A\rightarrow B}^{\Lambda} (|\psi\rangle) \). We recall that, due to the purity of the input and output states, a generic LOCC transformation which maps the vector \( |\psi\rangle \) in \( |\phi\rangle \) can always be realized via a single POVM on \( A \) followed by a unitary rotation on \( B \) conditioned by the measurement outcome, see e.g.

In other words, we can write

\[
|\phi\rangle\langle\phi| = \sum_{j} (M_{jA} V_{jB}) |\psi\rangle\langle\psi| (M_{jA}^\dagger V_{jB}^\dagger),
\]

where \( \{M_{jA}\} \) is a set of Kraus operators on \( A \) (\( \sum_{j} M_{jA}^\dagger M_{jA} = I_{A} \)), and \( \{V_{jB}\} \) is a set of unitary operators on \( B \). Introducing the set of probabilities \( \{p_{j}\} = \{\langle\psi|M_{jA}^\dagger M_{jA} |\psi\rangle\} \), from (14) it follows that for all \( j \) corresponding to \( p_{j} \neq 0 \) we must have

\[
M_{jA} V_{jB} |\psi\rangle = \sqrt{p_{j}} |\phi\rangle \quad \forall \ j \text{ s.t. } p_{j} \neq 0 .
\]

Observe also that for each \( H_{A}^{\Lambda} \), there exists an \( H_{B}^{\Lambda} \) which has the same components in the Schmidt basis of \( |\psi\rangle \), that is

\[
\langle\psi| e^{iH_{A}^{\Lambda}} \otimes I_{B} |\psi\rangle = \langle\psi| I_{A} \otimes e^{iH_{B}^{\Lambda}} |\psi\rangle .
\]

From equation (6) it follows then that for pure input states maximization over all \( H_{A}^{\Lambda} \) is equivalent to a maximization over all \( H_{B}^{\Lambda} \). This allows one to write

\[
D_{A\rightarrow B}^{\Lambda} (|\psi\rangle) = 1 - \max_{\{H_{B}^{\Lambda}\}} \left| \langle\psi| e^{iH_{A}^{\Lambda}} |\psi\rangle \right|^{2}
\]

\[
= 1 - \min_{\{H_{B}^{\Lambda}\}} \left| \langle\psi| e^{iH_{A}^{\Lambda}} |\psi\rangle \right|^{2}
\]

\[
= 1 - \left| \langle\psi| e^{iH_{B}^{\Lambda}} |\psi\rangle \right|^{2},
\]

where \( H_{B}^{\Lambda} \) labels the Hamiltonian for which the maximum is reached. Along the same lines, we have

\[
D_{A\rightarrow B}^{\Lambda} (|\phi\rangle) = 1 - \max_{\{H_{B}^{\Lambda}\}} \left| \langle\phi| e^{iH_{A}^{\Lambda}} |\phi\rangle \right|^{2}
\]

\[
= 1 - \sum_{j} \frac{1}{p_{j}} \max_{\{H_{B}^{\Lambda}\}} \left| \langle\psi|M_{jA}^\dagger M_{jA} e^{iH_{B}^{\Lambda}} |\psi\rangle \right|^{2},
\]
where the second identity follows from equation (15) by absorbing the unitary operator \( V_{jB} \) into the maximization over \( H_A^i \). The rhs of the latter expression can be bounded from above by noticing that the maximum of a given function is greater than the function evaluated at a given point. In particular we have

\[
D_{A-B}^A (|\phi\rangle) \leq 1 - \sum_i \frac{1}{p_j} \left| \langle \psi | M_A^j M_A^j e^{i\theta} | \psi \rangle \right|^2, \tag{20}
\]

where \( \tilde{H}_B^A \) has been introduced in equation (18). Finally, applying the Cauchy–Schwarz inequality we get

\[
D_{A-B}^A (|\phi\rangle) \leq 1 - \left| \langle \psi | \sum_j M_A^j M_A^j e^{i\theta} | \psi \rangle \right|^2 \\
= 1 - \left| \langle \psi | e^{i\tilde{H}_B^A} | \psi \rangle \right|^2 = D_{A-B}^A (|\psi\rangle), \tag{21}
\]

hence concluding the proof. \( \square \)

3.2. A formal connection between DS and LQU measures

The LQU measure of non-classical correlations was introduced in [23]. Given a state \( \rho \) of the bipartite system AB it can be computed as

\[
\mathcal{U}_{A-B}^A (\rho) = \min \mathcal{I} (\rho, H_A^i), \tag{22}
\]

where

\[
\mathcal{I} (\rho, H_A^i) := \text{Tr} \left( H_A^i \rho H_A^i - \sqrt{\rho} H_A^i \sqrt{\rho} H_A^i \right), \tag{23}
\]

is the Wigner–Yanase skew information [30] and where, as in equation (11), the maximum is taken over the set \( \{ H_A^i \} \) of the Hamiltonians (9). A connection between (22) and our DS measure follows by taking a formal expansion of equation (11) with respect to \( \Lambda \), i.e.

\[
D_{A-B}^A (\rho) = 1 - \max \min \text{Tr} \left[ \rho^s e^{i\tilde{H}_B^A} \rho^{1-s} e^{-i\tilde{H}_B^A} \right] \\
= - \max \min \text{Tr} \left[ \rho^s H_A^i \rho^{1-s} H_A^i - H_A^i \rho H_A^i \right] + O \left( \Lambda^3 \right) \\
= - \max \text{Tr} \left[ \sqrt{\rho} H_A^i \sqrt{\rho} H_A^i - H_A^i \rho H_A^i \right] + O \left( \Lambda^3 \right) \\
= \min \text{Tr} \left[ H_A^i \rho H_A^i - \sqrt{\rho} H_A^i \sqrt{\rho} H_A^i \right] + O \left( \Lambda^3 \right) \\
= \mathcal{U}_{A-B}^A (\rho) + O \left( \Lambda^3 \right), \tag{24}
\]

where in the third identity we used the following property.
Lemma 1. Given \( \rho \) a density matrix and \( \Theta = \Theta^\dagger \) a Hermitian operator we have

\[
\min_{0 \leq s \leq 1} \text{Tr} \left[ \rho^s \Theta \rho^{1-s} \Theta \right] = \text{Tr} \left[ \rho^{1/2} \Theta \rho^{1/2} \Theta \right].
\] (25)

Proof. Expressing \( \rho \) in terms of its eigenvectors \( \{ |\psi_\ell \rangle \} \) we can write

\[
\min_{0 \leq s \leq 1} \text{Tr} \left[ \rho^s \Theta \rho^{1-s} \Theta \right] = \sum_{\ell} c_\ell \left| \langle \psi_\ell | \Theta | \psi_{\ell'} \rangle \right|^2
\]

\[\quad + \min_{0 \leq s \leq 1} \sum_{\ell < \ell'} \left( c_\ell^s c_{\ell'}^{1-s} + c_{\ell'}^s c_\ell^{1-s} \right) \left| \langle \psi_\ell | \Theta | \psi_{\ell'} \rangle \right|^2,
\]

where \( \{ c_\ell \} \) are the eigenvalues of \( \rho \) organized in decreasing order (i.e. \( c_\ell \geq c_{\ell'} \) for \( \ell \leq \ell' \)). The thesis then follows by simply noticing that for all couples \( \ell < \ell' \), the functions \( f(s) = c_\ell^s c_{\ell'}^{1-s} + c_{\ell'}^s c_\ell^{1-s} \) reach their minima for \( s = 1/2 \) (indeed their first derivative \( f'(s) = (c_\ell^s c_{\ell'}^{1-s} - c_{\ell'}^s c_\ell^{1-s}) \ln(c_\ell/c_{\ell'}) \) are non-negative for \( s \geq 1/2 \) and non-positive for \( s \leq 1/2 \)).

Equation (24) establishes a formal connection between our DS measure and the LQU measure, providing hence a clear operational interpretation for the latter. Specifically the LQU can be seen as the DS measure of a discrimination process where \( \Lambda \) is a small quantity, i.e. where the allowed rotations \( \Lambda R \) of equation (10) are small perturbations of the identity operator. As we shall see in section 3.5, the relation between DS and LQU becomes even more stringent when \( \Lambda \) is a qubit system: indeed, in this special case, independently from the dimensionality of \( B \), the two measures are proportional.

3.3. Dependence upon \( \Lambda \)

According to section 3.1 all choices of matrix \( \Lambda \) in equation (8) provide a proper measure of non-classicality for the states \( \rho \). Even though one is tempted to conjecture that the case where \( \Lambda \) has an harmonic spectrum (i.e. \( \lambda_k - \lambda_{k-1} = \text{const} \) for all \( k = 2, 3, \ldots, d_\Lambda \)) should be somehow optimal (i.e. yield a more accurate measure of non-correlations), the relations among these different DSs at present are not clear and indeed it might be possible that no absolute ordering can be established among them (this is very much similar to what happens for the LQU [23]). Here we simply notice that since QCB is invariant under constant shifts in the local Hamiltonian spectrum, i.e. \( Q(\rho, e^{i\theta_1} \rho e^{-i\theta_1}) = Q(\rho, e^{i(\theta_1+\theta_2)} \rho e^{-i(\theta_1+\theta_2)}) \), for all incoming states \( \rho \) and for \( b \in \mathbb{R} \), we can always add a constant to \( \Lambda \) at convenience without affecting the corresponding DS measure, i.e.

\[
D^\Lambda_{\lambda-b}(\rho) = D^{\Lambda+b}_{\lambda-b}(\rho), \quad \forall \rho.
\] (26)
3.4. DS for pure states

Let $|\psi\rangle$ be a pure state of $AB$ with Schmidt decomposition [29] given by

$$|\psi\rangle = \sum_{j=1}^{\min[d_A,d_B]} \sqrt{q_j} |f_j\rangle_A |j\rangle_B ,$$

(27)

where $\{|f_j\rangle_A\}$ and $\{|j\rangle_B\}$ are orthonormal sets of $A$ and $B$, respectively ($d_{A,B}$ being the dimensionality of $A$, $B$). From equation (17) it follows that in this case the DS can be written as

$$D^A_{A\rightarrow B} (|\psi\rangle) = 1 - \max_{\{\mu\}} \left| \sum_j q_j A_j e^{i\mu_k} |j\rangle_A \right|^2$$

$$= 1 - \max_{\{\mu\}} \left| \text{Tr} \left[ \rho_A e^{i\mu_k} \right] \right|^2 ,$$

(28)

where $\rho_A = \text{Tr}_B [|\psi\rangle_A \langle \psi|]$ is the reduced state of $|\psi\rangle$ on $\mathcal{H}_A$. From the spectral decomposition (9) of $H^A_{\Lambda}$, one can perform the trace in (28) over the eigenbasis of $\Lambda$ and get

$$D^A_{A\rightarrow B} (|\psi\rangle) = 1 - \max_{\{M\}} \left| \sum_k \left( \sum_j M^{(k)}_j q_j \right) e^{i\lambda_k} \right|^2 ,$$

(29)

where now the maximization is performed over the set of the double stochastic matrices $M$ with elements $M^{(k)}_j = \lambda_k \langle U^A_{\Lambda} | j \rangle \langle j | U^A_{\Lambda} | k \rangle_A$. We recall that according to the Birkhoff theorem [31] $M$ can be written as a convex combination of permutation matrices $\Pi_\alpha$ (corresponding to the permutation $\pi_\alpha$), i.e.

$$B = \sum_\alpha p_\alpha \Pi_\alpha \quad \text{with} \quad \sum_\alpha p_\alpha = 1 .$$

(30)

Therefore, we can rewrite equation (29) as

$$D^A_{A\rightarrow B} (|\psi\rangle) = 1 - \max_{\{\mu\}, \{\ell\}} \left| \sum_{\alpha,k} p_\alpha \sum_j M^{(j)}_k q_j e^{i\lambda_k} \right|^2$$

$$= 1 - \max_{\{\mu\}, \{\ell\}} \left| \sum_\alpha p_\alpha \sum_k q_{\alpha,k} e^{i\lambda_k} \right|^2 .$$

(31)

Note that if $d_B < d_A$, the number of Schmidt coefficients is smaller than the number of eigenvalues $\lambda_k$. In this case, the expressions above hold as long as one considers the state (27) as having $d_A - d_B$ Schmidt coefficients equal to zero, i.e. one must apply the permutations to the set $\{q_1,...,q_{d_A}, q_{d_A+1} = 0,...,q_{d_B} = 0\}$.

By convexity it derives that the optimization over the set $\{p_\alpha\}$ in (31) can be explicitly carried out by choosing those probability sets $\{p_\alpha\}$ which have only a single element greater than zero (and thus equal to 1), from which we finally derive
where the maximization over the infinite set of Hamiltonians $H^A_i$ required by its definition (see equation (11)) has been replaced by a maximization over the group of permutations $\{\pi_\alpha\}$ on the set of the Schmidt coefficients $q_\alpha$.

### 3.4.1. Hamiltonians with harmonic spectrum

If the spectrum of the Hamiltonian $H^A_i$ is harmonic with fundamental frequency $\omega = |\lambda_i - \lambda_{i+1}| \leq 2\pi/d_A$, equation (32) can be further simplified. More precisely, let us relabel the set of eigenvalues $\{\lambda_i\}$ as

$$\lambda_1 = \omega, \quad \lambda_2 = -\omega, \quad \lambda_3 = -2\omega, \quad \lambda_4 = 2\omega, \quad \lambda_5 = -2\omega, \quad \text{etc},$$

yielding

$$D^A_{A-B} (|\psi\rangle) = 1 - \left| \sum_{k} d_{\alpha_k} e^{ik\omega} \right|^2,$$

(34)

3.5. DS for qubit–qudit systems

We conclude the section by considering the case in which subsystem $A$ is given by a single qubit, and determine a closed expression for the DS. Exploiting the gauge invariance (26) we set, without loss of generality, $\Lambda = \text{Diag} \{ -\lambda, \lambda \}$ and parameterize the set of local Hamiltonians acting on $A$ as $H^A_i = \hat{\lambda} \cdot \vec{\sigma}_A$, where $\hat{\lambda}$ is a unit vector in the Bloch sphere and $\vec{\sigma}_A = (\sigma_{A,1}, \sigma_{A,2}, \sigma_{A,3})$ is the vector formed by the Pauli operators. In what follows we will set $\sigma^{(\hat{\lambda})}_A = \hat{\lambda} \cdot \vec{\sigma}_A$. Under these hypotheses, the QCB can be written as

$$Q(\rho_0, \rho_1) = \min_{x \in [0,1]} \text{Tr} \left[ \rho^x e^{ix\sigma^{(\hat{\lambda})}_A} \rho^{1-x} e^{-ix\sigma^{(\hat{\lambda})}_A} \right]$$

$$= \cos^2 \lambda + \min_{x \in [0,1]} \text{Tr} \left[ \rho^x \sigma^{(\hat{\lambda})}_A \rho^{1-x} \sigma^{(\hat{\lambda})}_A \right] \sin^2 \lambda$$

$$= \cos^2 \lambda + \text{Tr} \left[ \rho^{1/2} \sigma^{(\hat{\lambda})}_A \rho^{1/2} \sigma^{(\hat{\lambda})}_A \right] \sin^2 \lambda,$$

where in the last equality we have used the fact that $\sigma^{(\hat{\lambda})}_A$ is Hermitian and lemma 1 to conclude that the minimization in $s$ is solved for $s = 1/2$ (see also footnote 5 on p 11 of [32]). Replacing this into equation (11) we finally obtain
\[ D_{A\rightarrow B}^A (\rho) = \max_{\tilde{\rho}} \left( 1 - \text{Tr}\left[ \rho^{1/2} \sigma^{(A)} \rho^{1/2} \sigma^{(A)} \right] \right) \sin^2 \lambda \]
\[ = \mathcal{U}_{A\rightarrow B}^A (\rho) \frac{\sin^2 \lambda}{\lambda^2} , \quad (35) \]

where
\[ \mathcal{U}_{A\rightarrow B}^A (\rho) = \lambda^2 \max_{\tilde{\rho}} \left( 1 - \text{Tr}\left[ \rho^{1/2} \sigma^{(A)} \rho^{1/2} \sigma^{(A)} \right] \right) , \quad (36) \]
is the LQU measure for a qubit–qudit system [23]—see equations (22) and (23). The identity (35) strengthens the formal connection between DS and LQU detailed in section 3.2 and provides a simple way to compute the DS for qubit–qudit systems. Indeed using the results of [23] it follows that
\[ D_{A\rightarrow B}^A (\rho) = \left[ 1 - \xi_{\text{max}} (W) \right] \sin^2 \lambda , \quad (37) \]
with \( \xi_{\text{max}} (W) \) being the maximum eigenvalue of a 3 × 3 matrix whose elements are given by
\[ W_{ij} = \text{Tr}\left[ \sqrt{\rho} \sigma_{i,j} \sqrt{\rho} \sigma_{i,j} \right] . \quad (38) \]
If \( \rho \) is pure, \( \rho = |\psi\rangle \langle \psi| \), the DS reduces to
\[ D_{A\rightarrow B}^A (|\psi\rangle) = \left[ 1 - (q_1 - q_0)^2 \right] \sin^2 \lambda , \quad (39) \]
where \( q_1 \) and \( q_2 \) are the Schmidt coefficients of \( |\psi\rangle \). In particular, notice that for separable pure states we have \( |q_1 - q_0| = 1 \) and the discord vanishes (see property 1 in section 3). On the other hand, for maximally entangled qubit–qudit states we have \( q_0 = q_1 = 1/2 \) and the DS reaches the maximum value \( \sin^2 \lambda \) (see property 4).

4. Maximization of the DS over the set of separable states

The main role played by the discord in the realm of quantum mechanics is enlightening the presence of those quantum correlations which cannot be classified as quantum entanglement. Here, we investigate the behavior of the DS when computed on the set of separable states \( \rho^{(\text{sep})} \) (yielding zero entanglement). We will prove that for all qubit–qudit systems (\( d_A = 2 \) and \( d_B \geq 2 \)), the maximum discord over the set of separable states is reached over the subset of pure \textit{quantum-classical} (pQC) states given by convex combinations of pure (non-necessarily orthogonal) states \( \{|\psi_k\rangle_A\} \) on \( A \) and orthonormal basis \( \{|k\rangle_B\} \) on \( B \), i.e.
\[ \rho^{(\text{pQC})} = \sum_k p_k |\psi_k\rangle_A \langle \psi_k| \otimes |k\rangle_B \langle k| , \quad (40) \]
the \( \{p_k\} \) being probabilities. For the case \( d_B \geq 3 \) we have an analytical proof of this fact, which allows us to solve the maximization and show that the following identity holds
\[ \max_{\rho^{(\text{sep})}} D_{A\rightarrow B}^A (\rho) = \max_{\rho^{(\text{pQC})}} D_{A\rightarrow B}^A (\rho) = \frac{2}{3} \sin^2 \lambda , \quad (41) \]
(see section 4.1 for the case \( d_B = \infty \) and section 4.2 for the case \( d_B \geq 3 \)). For \( d_B = 2 \) (i.e. for the qubit–qubit case) instead the optimality of the pure-QC states can only be verified numerically showing that

\[
\max_{\rho_{\text{sep}}} D_{A \rightarrow B}^A (\rho) = \max_{\rho_{\text{pQC}}} D_{A \rightarrow B}^A (\rho_{\text{pQC}}) = \frac{1}{2} \sin^2 \lambda, \tag{42}
\]

(see section 4.3).

### 4.1. p-QC states maximize the DS over the set of separable states: case \( d_B = \infty \)

A generic separable state can always be written as

\[
\rho_{\text{sep}} = \sum_k p_k | \psi_k \rangle_A \langle \psi_k | \otimes \rho_B^{(k)}, \tag{43}
\]

where \( \{ | \psi_k \rangle_A \} \) are (possibly non-orthogonal) pure states on \( \mathcal{H}_A \) and \( \{ \rho_B^{(k)} \} \) is a set of density matrices on \( \mathcal{H}_B' \), while \( \{ p_k \} \) are probabilities. From the joint concavity of the QCB (4) [24] and from the cyclic property of the trace, we have

\[
Q \left( \rho_{\text{sep}}, e^{i H_A} \rho_{\text{sep}}^\dagger e^{-i H_A} \right) \geq \sum_k p_k Q \left( | \psi_k \rangle_A \langle \psi_k | \otimes \rho_B^{(k)}, e^{i H_A} | \psi_k \rangle_A \langle \psi_k | e^{-i H_A} \otimes \rho_B^{(k)} \right)
= \sum_k p_k Q \left( | \psi_k \rangle_A \langle \psi_k |, e^{i H_A} | \psi_k \rangle_A \langle \psi_k | e^{-i H_A} \right)
= \sum_k p_k | \langle \psi_k | e^{i H_A} | \psi_k \rangle_A |^2. \tag{44}
\]

By direct calculation, one can easily verify that the above inequality is saturated a pure-QC state \( \rho_{\text{pQC}} \) of equation (40) obtained by replacing the density matrices \( \rho_B^{(k)} \) of (43) with orthogonal projectors \( | k \rangle_B \langle k | \) (notice that this is possible because \( B \) is infinite dimensional). Indeed in this case we have

\[
Q \left( \rho_{\text{pQC}}, e^{i H_A} \rho_{\text{pQC}}^\dagger e^{-i H_A} \right)
= \min_{0 \leq r \leq 1} \text{Tr} \left[ \left( \sum_k p_k | \psi_k \rangle_A \langle \psi_k | \otimes | k \rangle_B \langle k | \right)^r \left( \sum_k p_k e^{i H_A} | \psi_k \rangle_A \langle \psi_k | e^{-i H_A} \otimes | k' \rangle_B \langle k' | \right)^{1-r} \right]
= \sum_k p_k | \langle \psi_k | e^{i H_A} | \psi_k \rangle_A |^2. \tag{45}
\]

Since \( Q \left( \rho_{\text{sep}}, e^{i H_A} \rho_{\text{sep}}^\dagger e^{-i H_A} \right) \) is greater than \( Q \left( \rho_{\text{pQC}}, e^{i H_A} \rho_{\text{pQC}}^\dagger e^{-i H_A} \right) \) for each choice of \( H_A' \), we conclude that

\[
D_{A \rightarrow B}^A (\rho_{\text{sep}}) \leq D_{A \rightarrow B}^A (\rho_{\text{pQC}}). \tag{46}
\]

Next we show that the maximum DS attainable over the set of pQC states (and hence over the set of separable states) cannot be larger than \( \frac{2}{3} \sin^2 \lambda \). To do so let us first consider the uniform pQC state \( \rho_{\text{pQC}}^{(n)} \),
\[ \rho_{\text{pQC}}^{(\text{pQC})} = \frac{1}{d} \sum_{j=0}^{d-1} |\psi_j\rangle_A \langle \psi_j| \otimes |j\rangle \langle j|, \]  

characterized by \( d \) pure states \( \{ |\psi_j\rangle_A \} \) whose corresponding vectors \( \{ \hat{r}_j \} \) in the Bloch sphere are assumed to be uniformly distributed (i.e. their \( d \) vertices identify a regular polyhedron). From equation (45) we have

\[
D_{A \rightarrow B}^{(\text{pQC})} (\rho_{\text{pQC}}^{(\text{pQC})}) = \min_{\{n^A\}} \sum_{j=0}^{d-1} \frac{1}{d} \left( 1 - |\langle \psi_j| e^{jH^A_n} |\psi_j\rangle_A|^2 \right)
\]

\[
= \min_{\{n\}} \sum_{j=0}^{d-1} \frac{1}{d} \left[ 1 - \cos^2 \lambda - \sin^2 \lambda \left( \hat{r}_j \cdot \hat{n} \right)^2 \right]
\]

\[
= \left( 1 - \max_{\{n\}} \frac{1}{d} \sum_{j=0}^{d-1} \cos^2 \theta_j \right) \sin^2 \lambda , \tag{48}
\]

where we set \( H^A_n = \lambda \sigma_A^{(n)} \) (see section 3.5) and introduced \( \cos \theta_j = \hat{n} \cdot \hat{r}_j \). In the limit \( d \rightarrow \infty \) the series \( \sum_{j=1}^{d} \cos^2 \theta_j \) converges to an integral over the solid angle, which does not depend on the orientation of \( \hat{n} \), i.e.

\[
\lim_{d \rightarrow \infty} \frac{1}{d} \sum_{j=0}^{d-1} \cos^2 \theta_j = \frac{1}{4\pi} \int d\Omega \cos^2 \theta
\]

\[
= \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \cos^2 \theta = \frac{1}{3} . \tag{49}
\]

Therefore we have

\[
D_{A \rightarrow B}^{(\text{pQC})} (\rho_{\text{pQC}}^{(\text{pQC})}) = \frac{2}{3} \sin^2 \lambda . \tag{50}
\]

To prove that the above quantity is also the maximum value of DS over the whole set of pure-QC states (40) we notice that, proceeding as in equation (48), we can write

\[
D_{A \rightarrow B}^{(\text{pQC})} (\rho^{(\text{pQC})}) = \left( 1 - \max_{\{n\}} \sum_{j=0}^{d-1} p_j (\hat{r}_j \cdot \hat{n})^2 \right) \sin^2 \lambda
\]

\[
= \left( 1 - \sum_{j=0}^{d-1} p_j (\hat{r}_j \cdot \hat{n}_a)^2 \right) \sin^2 \lambda , \tag{51}
\]

where \( \hat{n}_a \) indicates the direction which saturates the maximization. This vector is clearly a function of the state \( \rho^{(\text{pQC})} \), i.e. it depends both on the probabilities \( p_j \) and on the vectors \( \hat{r}_j \). If we define the state \( \rho_R^{(\text{pQC})} \), obtained from \( \rho^{(\text{pQC})} \) by applying to the vectors \( \hat{r}_j \) a rotation matrix \( R \in SO(3) \), we have

\[
D_{A \rightarrow B}^{(\text{pQC})} (\rho_R^{(\text{pQC})}) = D_{A \rightarrow B}^{(\text{pQC})} (\rho^{(\text{pQC})}) , \tag{52}
\]
where the vector saturating the maximization in equation (51) now corresponds to $R\hat{n}_B$. By introducing an ancillary system $C$, associated to the Hilbert space $\mathcal{H}_C$, and a set of $N$ 3D-rotations $\{R_k\}$, mapping each vertex of the regular N-polyhedron on all vertices (including itself), one can define the density matrix

$$
\rho^{(pQC)}_{ABC} := \frac{1}{N} \sum_{k=0}^{N-1} \sum_{j=0}^{d-1} p_j \left| \psi_j (R_k) \right\rangle \left\langle \psi_j (R_k) \right| \bigotimes_j \left| j \right\rangle_B \bigotimes_k \left| k \right\rangle_C \bigotimes_k \left| k \right\rangle.
$$

where

$$
\rho^{(pQC)}_{A,C} := \frac{1}{N} \sum_{k=0}^{N-1} \rho^{(pQC)}_{R_k} \bigotimes_k \left| k \right\rangle_C \bigotimes_k \left| k \right\rangle.
$$

On the other hand $\tilde{\rho}^{(pQC)}_{ABC}$ can also be arranged as

$$
\tilde{\rho}^{(pQC)}_{ABC} = \sum_{j=0}^{d-1} p_j \rho^{(pQC)}_{R_{u,n,j}} \bigotimes_j \left| j \right\rangle_B \bigotimes_j \left| j \right\rangle.
$$

where the density matrices $\rho^{(pQC)}_{R_{u,n,j}}$, on $\mathcal{H}_A \otimes \mathcal{H}_C$, are defined as

$$
\rho^{(pQC)}_{R_{u,n,j}} := \frac{1}{N} \sum_{k=0}^{N-1} \left| \psi_j (R_k) \right\rangle \left\langle \psi_j (R_k) \right| \bigotimes_k \left| k \right\rangle_C \bigotimes_k \left| k \right\rangle.
$$

It is important to observe that since $B$ is infinite dimensional, there always exists a state $\hat{\rho}^{(pQC)}_{ABC}$ of $AB$ which is fully isomorphic to $\rho^{(pQC)}_{ABC}$, from which it follows

$$
Q \left( \hat{\rho}^{(pQC)}_{ABC}, \hat{n} \right) = Q \left( \rho^{(pQC)}_{ABC}, \hat{n} \right),
$$

where

$$
Q \left( \rho, \hat{n} \right) := Q \left( \rho, e^{i\hat{a}^{(n)}} \rho e^{-i\hat{a}^{(n)}} \right).
$$

Thanks to expansion (53), we get

$$
Q \left( \hat{\rho}^{(pQC)}_{ABC}, \hat{n} \right) = \frac{1}{N} \sum_{k=0}^{N-1} Q \left( \rho^{(pQC)}_{R_k}, \hat{n} \right).
$$

from which, taking the maximum over $\hat{n}$, it results

$$
\max_{\hat{n}} \sum_{k=0}^{N-1} Q \left( \rho^{(pQC)}_{R_k}, \hat{n} \right) \leq \sum_{k=0}^{N-1} \max_{\hat{n}} Q \left( \rho^{(pQC)}_{R_k}, \hat{n} \right).
$$

Finally, since for all $k$, $\rho^{(pQC)}_{R_k}$ and $\rho^{(pQC)}_{R_k}$ share the same DS (see equation (52)), we get

$$
D_{A \rightarrow B}^{\hat{\rho}^{(pQC)}}(\hat{\rho}^{(pQC)}) \geq D_{A \rightarrow B}^{\rho^{(pQC)}}(\rho^{(pQC)}).
$$
On the other hand, thanks to expansion (55) we have

$$Q\left(\hat{\rho}^{(pQC)}, \hat{n}\right) = \sum_{j=0}^{d-1} p_j Q\left(\rho_{u,N,j}^{(pQC)}, \hat{n}\right),$$

and therefore

$$\max_{[\hat{n}]} Q\left(\hat{\rho}^{(pQC)}, \hat{n}\right) \leq \sum_{j=0}^{d-1} p_j \max_{[\hat{n}]} Q\left(\rho_{u,N,j}^{(pQC)}, \hat{n}\right).$$

The above inequality is saturated in the limit $N \to \infty$, where each $\rho_{u,N,j}^{(pQC)}$ approaches the state $\rho_{u,\infty}^{(pQC)}$ characterized by

$$Q\left(\rho_{u,\infty}^{(pQC)}, \hat{n}\right) = \cos^2 \lambda - \frac{1}{3} \sin^2 \lambda, \quad \forall \hat{n}$$

(see equation (50)). We therefore have

$$D_{A-B}^{\lambda} \left(\rho_{u,\infty}^{(pQC)}\right) = \sum_{j=0}^{d-1} p_j \frac{2}{3} \sin^2 \lambda = \frac{2}{3} \sin^2 \lambda.$$

The identity (41) finally follows by combining equations (46), (61) and (65).

### 4.2. p-QC states maximize the DS over the set of separable states: case $d_B \geq 3$

If $\mathcal{H}_B$ is finite dimensional we are not guaranteed about the possibility of mapping a generic separable state in a pure-QC state. Thus relation (46) could be in principle violated. However by embedding $\mathcal{H}_B$ into a larger system having infinite dimension one can still invoke the result of the previous subsection to say that

$$\max_{\rho^{(\text{sep})}} D_{A-B}^{\lambda} \left(\rho^{(\text{sep})}\right) \leq \frac{2}{3} \sin^2 \lambda.$$

To prove equation (41) it is hence sufficient to produce an example of a pure-QC state (40) that reaches such an upper bound. Of course the sequence of uniform states (47) cannot be used for this purpose because now $d_B$ is explicitly assumed to be finite. Instead we take

$$\rho^{(pQC)} = \sum_{j=0,1,2} p_j \left| \psi_j \right\rangle_A \left\langle \psi_j \right| \otimes \left| j \right\rangle_B \left\langle j \right|,$$

with $\left| 0 \right\rangle_B, \left| 1 \right\rangle_B, \left| 2 \right\rangle_B$ being orthonormal elements of $\mathcal{H}_B$, which is a properly defined p-QC state whenever the dimension $d_B$ is larger than 3. As in the first line of equation (51), its associated DS can then be computed as,

$$D_{A-B}^{\lambda} \left(\rho^{(pQC)}\right) = \left(1 - \max_{\hat{n}} \sum_{j=0}^{2} p_j (\hat{r}_j \cdot \hat{n})^2\right) \sin^2 \lambda,$$

where $\hat{r}_j$ is the vector in the Bloch sphere of the state $|\psi_j\rangle$ while $H_A^{\lambda} = \lambda A^{(\hat{r})}$. We are interested in the case where $\{\hat{r}_j\}$ is an orthonormal triplet (i.e. the three vectors identifying three Cartesian axes in the 3D-space). Notice that this does not mean that the corresponding states are
orthogonal: instead they are mutually unbalanced states (e.g. \( |\psi_0\rangle_A = |0\rangle_A \), \( |\psi_1\rangle_A = |+\rangle_A = (|0\rangle_A + |1\rangle_A)/\sqrt{2} \), \( |\psi_2\rangle_A = |\times\rangle_A = (|0\rangle_A + i |1\rangle_A)/\sqrt{2} \)), so that (67) corresponds to an (unbalanced) generalized B92 (GB92) state. From the normalization condition on vector \( \hat{n} \), it derives that the squared scalar products \((\hat{n} \cdot \hat{r}_j)^2\) define a set of probabilities, since
\[
\sum_{j=0,1,2} (\hat{n} \cdot \hat{r}_j)^2 = |\hat{n}|^2 = 1. \tag{69}
\]
Thus, the maximization involved in (68) can be trivially performed by choosing \( \hat{n} \) parallel to the \( \hat{r}_j \) associated to the maximum weight \( p_j \). This gives
\[
D_{A \rightarrow B}^A(\rho^{(GB92)}) = \left( 1 - \max \left\{ p_0, p_1, p_2 \right\} \right) \sin^2 \lambda. \tag{70}
\]
By observing that for a three event process the maximum probability can never be smaller than \( 1/3 \), we conclude that the maximum DS over the set of GB92 states is achieved by the equally weighted (EW) one
\[
\rho^{(GB92)}_{EW} = \frac{1}{3} \left( |0\rangle_A \langle 0| \otimes |0\rangle_B \langle 0| + |+\rangle_A \langle +| \otimes |1\rangle_B \langle 1| + |\times\rangle_A \langle \times| \otimes |2\rangle_B \langle 2| \right). \tag{71}
\]
With this choice we get
\[
D_{A \rightarrow B}^A(\rho^{(GB92)}_{EW}) = \frac{2}{3} \sin^2 \lambda, \tag{72}
\]
which shows that, also for \( d_B \) finite and larger than 3, the upper bound (66) is achievable with a pure-QC state, hence proving (41).

4.3. p-QC states maximize the DS over the set of separable states: case \( d_B = 2 \) (qubit–qubit)

The argument used in the previous section cannot be directly applied to analyze the qubit–qubit case (i.e. \( d_A = d_B = 2 \)), because for those systems the states (67) and (71) cannot be defined. Furthermore we will see that the upper bound (66) is no longer tight. To deal with this case we first consider the class of QC state and show that the maximum of DS, equal to \((1/2) \sin^2 \lambda\), is achieved on the set of pure QC states. Then we resort to numerical optimization procedures to show that no other separable qubit–qubit state can do better than this, hence verifying the identity (42).

4.3.1. Maximum DS over QC states. A generic QC state for the qubit–qubit case can be expressed as

\[\text{These are indeed the two-qubit states (or their generalization to qubit–qutrit systems) used in the Bennett-92 protocol for quantum cryptography [Bennett C H 1992 Phys. Rev. Lett. 68 31213124] if one uses the first qubit to encode the message (0 \( \rightarrow \) |0\rangle, 1 \( \rightarrow \) |+\rangle), i.e. this is the qubit that is actually sent from Alice to Bob, and the second qubit to keep track of the message (0 \( \rightarrow \) |0\rangle, 1 \( \rightarrow \) |1\rangle), i.e. this is a classical register of what has been sent.} \]
\[ \rho^{(\text{OC})} = p \, \tau_0 \otimes |0\rangle_\beta \langle 0| + (1 - p) \, \tau_1 \otimes |1\rangle_\beta \langle 1|, \]  

(73)

where \( p \in [0, 1] \), \( \tau_0 \) and \( \tau_1 \) are generic mixed states of \( A \), and \( \{ |0\rangle_\beta, |1\rangle_\beta \} \) is an orthonormal basis of \( \mathcal{H}_\beta \). To compute the associated value of DS we invoke equation (37) and determine the maximum eigenvalue of the matrix \( W_{\phi \theta} \) of equation (35). Recalling the invariance of DS under local unitary operations we then set

\[ \tau_0 = \frac{I + s_0 \sigma_3}{2}, \quad \tau_1 = \frac{I + s_1 \left( \sin \phi \, \sigma_1 + \cos \phi \, \sigma_3 \right)}{2}, \]  

(74)

with \( 0 \leq \phi \leq \pi \) and \( 0 \leq s_i \leq 1 \), which yields

\[ \sqrt{\epsilon_i} = R \left( \phi_i \right) \, A \left( s_i \right) + B \left( s_i \right) \, R^\dagger \left( \phi_i \right), \]  

(75)

where \( \phi_0 = 0 \), \( \phi_1 = \phi \), \( R \left( \theta \right) = \exp \left[ -i \frac{\theta}{2} \sigma_2 \right] \) and

\[ A \left( s_i \right) = \frac{\sqrt{1 + s_i} + \sqrt{1 - s_i}}{2}, \quad B \left( s_i \right) = \frac{\sqrt{1 + s_i} - \sqrt{1 - s_i}}{2}. \]  

(76)

We now have all the ingredients necessary for the computation of the matrix elements \( W_{\phi \theta} \).

Thanks to the orthogonality of \( |0\rangle_\beta \) and \( |1\rangle_\beta \), this gives

\[ W_{2\phi} = W_{\phi 2} = \left[ p \sqrt{1 - s_0^2} + (1 - p) \sqrt{1 - s_1^2} \right] \delta_{2\phi} > 0, \]

\[ W_{11} = p \sqrt{1 - s_0^2} + \frac{(1 - p)}{2} \left[ 1 - \cos \left( 2\phi \right) + \sqrt{1 - s_1^2} \left( 1 + \cos \left( 2\phi \right) \right) \right] > 0, \]

\[ W_{13} = W_{31} = (1 - p) \left( 1 - \sqrt{1 - s_1^2} \right) \sin \phi \cos \phi, \]

\[ W_{33} = \frac{1 + p}{2} + \frac{1 - p}{2} \left[ \cos \left( 2\phi \right) + \sqrt{1 - s_1^2} \left( 1 - \cos \left( 2\phi \right) \right) \right]. \]  

(77)

It derives that the eigenvalues of \( W \) reduce to

\[ \xi_0 = W_{22}, \]

\[ \xi_\pm = \frac{W_{11} + W_{33}}{2} \pm \frac{1}{2} \sqrt{(W_{11} - W_{33})^2 + 4W_{13}^2}. \]

Being \( W_{13} < 1 \) and \( W_{11} + W_{33} = 1 + W_{22} \), we have that \( \xi_+ \) is the maximum eigenvalue. Therefore equation (37) yields

\[ D_{A-B}^A \left( \rho^{(\text{OC})} \right) = f_w \, \frac{\sin^2 \lambda}{2}, \]  

(78)
where

\[ f_w := 1 - W_{22} - \sqrt{(W_{11} - W_{33})^2 + 4W_{13}^2} \]  

(79)

It derives

\[ D^A_{A-B}(\rho^{\text{QC}}) \leq \frac{\sin^2 \lambda}{2}, \]  

(80)

the equality being saturated when \( W_{22} = 0, W_{13} = 0 \) and \( W_{11} - W_{33} = 0 \). The first condition sets to 1 the purity of \( \tau_0 \) and \( \tau_1 \) \((s_0^2 = s_1^2 = 1)\), the second and third conditions imply \( \phi = (2n + 1)\pi/2 \), with \( n \in \mathbb{Z} \), and \( p = 1/2 \). We conclude that the maximum of the DS on the set of QC states is achieved on B92-like states, which are pure-QC, that is

\[ \text{max}_{\rho^{\text{QC}}} D^A_{A-B}(\rho^{(\text{QC})}) = D^A_{A-B}(\rho^{(\text{B92})}) = \frac{\sin^2 \lambda}{2}, \]  

(81)

being

\[ \rho^{(\text{B92})} = \frac{1}{2} \left( |0\rangle_A \langle 0| \otimes |0\rangle_B \langle 0| + |\sin(\phi)\rangle_A \langle \sin(\phi)| \otimes |1\rangle_B \langle 1| \right). \]  

(82)

and \( \sin(\phi) = \pm 1 \) and \( |\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2} \).

### 4.3.2. Separable qubit–qubit states: numerical results.

We conclude our analysis by providing numerical evidence that \((1/2) \sin^2 \lambda \) is the maximum value reached by the DS over all the sets of separable states as anticipated in equation (42). We recall that a generic separable state of two qubit systems can always be written as a finite convex sum of direct products of pure states for \( A \) and \( B \) \([33]\), i.e.

\[ \rho^{\text{sep}} = \sum_{j=1}^{N} p_j |\psi_j\rangle_A \langle \psi_j| \otimes |\chi_j\rangle_B \langle \chi_j|, \quad p_j > 0 \quad \forall \ j, \]  

(83)

with \( 1 \leq N \leq 4 \). We remark that here no orthogonality constraint has to be imposed on either sets of pure states \( \left\{ |\psi_j\rangle_A \right\} \) and \( \left\{ |\chi_j\rangle_B \right\} \), on \( \mathcal{H}_A \) and \( \mathcal{H}_B \), respectively. The Bloch sphere formalism allows us to define, for all \( j \)

\[ |\psi_j\rangle_A \langle \psi_j| = \frac{\mathbb{1} + \hat{\psi}_j \cdot \hat{\sigma}_A}{2} \quad \text{and} \quad |\chi_j\rangle_B \langle \chi_j| = \frac{\mathbb{1} + \hat{\chi}_j \cdot \hat{\sigma}_B}{2}. \]  

(84)

Summarizing, all qubit–qubit separable states are characterized by a set of \( N \) probabilities and \( 2N \) vectors of unit norms.

The case \( N = 1 \) is trivial (all separable states are completely uncorrelated) and the DS is always zero. Therefore, we have numerically analyzed the cases \( N = 2, N = 3 \) and \( N = 4 \) and plot our results in figure 2. The reported results are in agreement with equation (42).

The details of this numerical analysis are presented in appendix B.
5. Conclusions

In this paper we have introduced, under the name of DS, a novel measure of discord-like correlations, i.e. correlations that, even though they are not addressable as quantum entanglement, are still non-classical. In the *mare-magnum* of definitions and measures [1], each stemming from a different way in which quantum correlations can be used to outperform purely classical systems, the DS finds its natural collocation in the context of state discrimination. More precisely, it quantifies the ability of a given bipartite probing state to discriminate between the application or not of a unitary map to one of its two subsystems, when a large number of copies of the probing state is at disposal. We report that in a similar context, the noisy quantum illumination [19], a recent paper [34] has put forward a connection between the advantage yielded by quantum illumination over the best conceivable classical approach, and the amount of quantum discord (as in Ollivier and Zurek [3]) surviving in a maximally entangled state after the interaction with a noisy environment. Here however, our goal was to define a quantity which has a clear operative meaning (characterizing quantitatively each bipartite state as a resource for a specific task) and is also easy to compute, at least in some simple cases.

Specifically, we have proved that the DS fits all the requirements ascribing it as a proper measure of quantum correlations [1]. We have also provided a closed expression of this measure for some special cases, such as pure states and qubit–qudit systems. For the latter case we have also shown an explicit connection with another measure of quantum correlations, the LQU [23], which, in the most general case, can be seen to approximate the DS in the limit where the unitary map is close to the identity. Next, we have focused on the class of separable states and proved, by means of both analytical and numerical methods, that for all qubit–qudit systems the DS reaches its maximum on the set of pQC states. Finally, we have explicitly determined this maximum value.

We remind the reader that by definition the DS depends on the spectral properties of the encoding Hamiltonian $H_A$. In other words, for each specific choice of $A$ one can in principle define a different measure of quantum correlations (a similar problem also affects the LQU). It would be therefore interesting to investigate if there exists a criterion for comparing different measures arising from different spectral properties of $H_A$.

To conclude, we remark that the DS can be related to other discord-like measures that have been recently introduced, including the interferometric power [22], the LQU [23] and the DR [28]. Ultimately, all these measures share a common message: discord-like correlations are the fundamental resource to be used in many quantum metrology tasks. Moreover, the functionals on which they are based (Chernoff bound, Fisher information, Bures distance) are all interconnected, so that each measure could be used to bound the others [24, 32, 35]. Most interestingly, even the Bures geometric quantum discord, which stems from a different perspective, has been recently shown to be related to an ambiguous state discrimination problem [12]. In this perspective, we believe that our analysis marks a further step towards a novel classification of a vast set of non-classicality measures.
Acknowledgments

We thank G Adesso, D Girolami, F Illuminati and T Tufarelli for useful comments and discussions. ADP acknowledges support from Progetto Giovani Ricercatori 2013 of SNS.

Appendix A. Pedagogical remark

In this appendix, we provide an explicit proof that an arbitrary qubit–qutrit pQC state (67) cannot achieve a DS greater than $(2/3)\sin^2\lambda$. Note that this result naturally derives from what is found in sections 4.1 and 4.2. Nonetheless, we report the following proof as a pedagogical remark for the interested reader.

Consider an arbitrary qubit–qutrit pQC state (67) with strictly positive probabilities $\{p_j\}$ and with vectors $\{\hat{r}_j\}$ lying in the Bloch sphere. Without loss of generality we assume that $p_2 \geq p_1 \geq p_0$ and introduce a Cartesian coordinate set formed by the 3D orthonormal vectors $\{\hat{s}_j\}$ such that

$$\hat{r}_2 = \hat{s}_2, \quad \hat{r}_1 = \cos \theta \hat{s}_2 + \sin \theta \hat{s}_1, \quad \hat{r}_0 = \cos \theta' \hat{s}_2 + \sin \theta' \cos \phi' \hat{s}_0 + \sin \theta' \sin \phi' \hat{s}_1. \quad (A1)$$

See figure 3. With this choice we can write

$$\sum_{j=0,1,2} p_j (\hat{n} \cdot \hat{r}_j)^2 = \sum_{j=0,1,2} \tilde{p}_j \cos^2 \phi_j + \Delta (\phi_0, \phi_1, \phi_2), \quad (A2)$$

where $\phi_j$ is the angle between $\hat{n}$ and the Cartesian $j$th axis $\hat{s}_j$,

$$\cos \phi_j = \hat{n} \cdot \hat{s}_j, \quad (A3)$$
\( \{ \tilde{p}_j \} \) is still a probability set of elements

\[
\begin{align*}
\tilde{p}_2 &= p_2 + p_1 \cos^2 \theta + p_0 \cos^2 \theta', \\
\tilde{p}_1 &= p_1 \sin^2 \theta + p_0 \sin^2 \theta' \sin^2 \phi', \\
\tilde{p}_0 &= p_0 \sin^2 \theta' \cos^2 \phi',
\end{align*}
\]

(A4)

and \( \Delta \left( \phi_0, \phi_1, \phi_2 \right) \) is the function

\[
\begin{align*}
\Delta \left( \phi_0, \phi_1, \phi_2 \right) &= A \cos \phi_2 \cos \phi_1 + B \cos \phi_2 \cos \phi_0 + C \cos \phi_0 \cos \phi_1, \\
A &= p_1 \sin 2\theta + p_0 \sin 2\theta' \sin \phi', \\
B &= p_0 \sin 2\theta' \cos \phi', \\
C &= p_0 \sin^2 \theta' \sin 2\phi'.
\end{align*}
\]

(A5)

Observe that all the dependence of (A2) upon \( \hat{n} \) relies on the phases \( \{ \phi_j \} \): in particular the probabilities \( \{ \tilde{p}_j \} \) and the quantity \( A, B, \) and \( C \) of equation (A5) do not depend on the choice of the Hamiltonian: they only depend on the initial state (67). According to (68), in order to compute the DS of the state we need to find the maximum value of (A2) over all possible choices of \( \hat{n} \), i.e. for all possible coordinate components (A3). To do so we first use the following facts to show that it is always possible to have \( \Delta \) positive while keeping the first contribution of (A2) positive (i.e. \( \sum_{j=0,1,2} \tilde{B}_j \cos^2 \phi_j \geq 0 \)):

F1: given three real numbers \( a, b \) and \( c \), at least one of the four combinations must be non-negative, i.e. \( a + b + c, a - b - c, -a + b - c, -a - b + c \) (observe that their sum is null);
F2: The vectors which with respect to \( \hat{s}_j \) have coordinates
\[
\hat{n}_1 := (\cos \phi_0, \cos \phi_1, \cos \phi_2),
\]
\[
\hat{n}_2 := (-\cos \phi_0, \cos \phi_1, \cos \phi_2),
\]
\[
\hat{n}_3 := (\cos \phi_0, -\cos \phi_1, \cos \phi_2),
\]
\[
\hat{n}_4 := (\cos \phi_0, \cos \phi_1, -\cos \phi_2),
\]
have the same value of \( \sum_{j=0,1,2} \tilde{p}_j \cos^2 \phi_j \) but are associated to the following values for \( \Delta \phi_j \):
\[
\hat{n}_1 \rightarrow \Delta = a + b + c,
\]
\[
\hat{n}_2 \rightarrow \Delta = a - b - c,
\]
\[
\hat{n}_3 \rightarrow \Delta = -a + b - c,
\]
\[
\hat{n}_4 \rightarrow \Delta = -a - b + c,
\]
with \( a = A \cos \phi_2 \cos \phi_1, \ b = B \cos \phi_2 \cos \phi_0, \) and \( c = C \cos \phi_0 \cos \phi_1 \). From F1 it derives that at least one of the vectors \( \hat{n}_{1,2,3,4} \) will have positive \( \Delta \).

We therefore conclude that
\[
\max_{\hat{n}} \sum_{j=0,1,2} p_j (\hat{n} \cdot \hat{r}_j)^2 \geq \max_{\tilde{p}_j} \sum_{j=0,1,2} \tilde{p}_j \cos^2 \phi_j = \max \{ \tilde{p}_0, \tilde{p}_1, \tilde{p}_2 \},
\]
where the last identity follows from the fact that \( \{ \cos^2 \phi_j \} \) is a probability set, since it fulfills the normalization condition \( \sum_{j=0,1,2} \cos^2 \phi_j = 1 \), see equation (A3). Replacing this into equation (68) finally yields
\[
D_{A \rightarrow B}^{A-\rho (\rho^{Q(\psi)})} \leq \left( 1 - \max \{ \tilde{p}_0, \tilde{p}_1, \tilde{p}_2 \} \right) \sin^2 \lambda, \leq \frac{2}{3} \sin^2 \lambda,
\]
where the last inequality holds because the largest of three positive quantities summing to 1 cannot be smaller than 1/3.

Appendix B. Numerical analysis for qubit–qubit separable states

This appendix is devoted to discussing in deeper detail the numerical analysis presented in section 4.3.2.

We have computed the DS of a two-qubit system in an arbitrary separable state, which, without loss of generality can be written as
\[
\rho^{(\text{sep})} = \sum_{j=1}^{N} p_j \frac{\mathbb{I} + \hat{u}_j \cdot \hat{s}_A}{2} \otimes \frac{\mathbb{I} + \hat{v}_j \cdot \hat{s}_B}{2}, \quad p_j > 0 \quad \forall \ j,
\]
with \( 1 \leq N \leq 4 \), and \( \hat{u}_j, \hat{v}_j \) normalized vectors in the Bloch sphere [33].
Let us start with the case $N = 2$. The set of probabilities $\{p_i\}$ can be labelled as
\[
\{p_1, p_2\} = C_2 \{\sin \alpha, \cos \alpha\},
\]
\[
C_2 = \frac{1}{\sin \alpha + \cos \alpha},
\]
with $0 < \alpha \leq \pi/4$. The latter constraint implies $0 < p_1 \leq p_2$. Similarly, we have parameterized the unit vectors $\hat{u}_j$ and $\hat{v}_j$ by means of the polar and azimuthal angles, $0 \leq \theta^u_j \leq \pi$ and $0 \leq \phi^u_j < 2\pi$, respectively. For each angle, we have taken a set of uniformly distributed values within the corresponding range, and perform all possible combinations. Finally, we have set some additional constraints in the numerical code in order get rid of those states which are equivalent under local unitary transformations. Thanks to this procedure, we have generated a set of $\sim 7 \times 10^8$ separable states and found that the state with maximum DS corresponds to the B92 state (82) with $D_{A\rightarrow B}^\lambda = 1/2 \sin^2(\lambda \phi)$, thus confirming what is shown in section 4.3.

We have repeated the same analysis for the case $N = 3$ by setting
\[
\{p_1, p_2, p_3\} = C_3 \{\sin \alpha \sin \beta, \sin \alpha \cos \beta, \cos \alpha\},
\]
\[
C_3 = \frac{1}{\sin \alpha (\sin \beta + \cos \beta) + \cos \alpha},
\]
with $0 < \alpha, \beta \leq \pi/4$ to ensure that $0 < p_1 \leq p_2 \leq p_3$. We thus generated a set of $\sim 2 \times 10^6$ separable states. The maximum DS detected within this ensemble is $\sim 0.485 \sin^2 (\lambda \phi)$, and corresponds to
\[
\alpha = 3\pi/16, \quad \beta = \pi/4,
\]
\[
\theta^u_j = \phi^u_j = 0, \quad \theta^v_j = \pi/2, \quad \theta^v_j = \pi, \quad \phi^v_j = 0.
\]
Up to local unitary transformations, this set of parameters describes the state
\[
\rho^{(sep)} \approx 0.486 |0\rangle_A \langle 0 | 0 \rangle_B \langle 0 | + 0.514 |1\rangle_A \langle 1 | 0 \rangle_B \langle 1 |, \]
which is almost equivalent to the B92 state (82) found for $N = 2$. We foresee that, by means of a finer graining of the parameter space, one should be able to include in the ensemble generated with this procedure the B92 state and reach $1/2 \sin^2 (\lambda \phi)$ as the highest value for DS.

Finally we considered the case $N = 4$, which corresponds to setting in equation (B1)
\[
\{p_1, p_2, p_3, p_4\} = C_4 \{\sin \alpha \sin \beta \sin \gamma, \sin \alpha \sin \beta \cos \gamma, \sin \alpha \cos \beta, \cos \alpha\},
\]
\[
C_4 = \sin \alpha (\sin \beta (\sin \gamma + \cos \gamma) + \cos \beta) + \cos \alpha,
\]
with $0 < \alpha, \beta, \gamma \leq \pi/4$ ensuring $0 < p_1 \leq p_2 \leq p_3 \leq p_4$. We have thus generated a set of $\sim 10^6$ separable states. The maximum value we have found for the DS is $\sim 0.484 \sin^2 (\lambda \phi)$, achieved when
\[ \alpha = \pi/4, \beta = \pi/8, \gamma = \pi/4, \]
\[ \theta_j^{uv} = 0, \phi_j^{uv} = 0, \quad \text{for } j = 1, 4, \]
\[ \theta_k^{uv} = \pi/2, \quad \phi_k^{uv} = 0, \quad \text{for } k = 2, 3. \quad (B7) \]

This set of parameters defines the state
\[ \rho^{(\text{sep})} \approx 0.515 \left| 0 \right>_A \left\langle 0 \right|_B \otimes \left| 0 \right>_B \left\langle 0 \right| + 0.485 \right| 1 \right>_A \left\langle 1 \right|_B \otimes \left| 1 \right>_B \left\langle 1 \right|, \quad (B8) \]

which again, up to numerical errors, is quite close to the aforementioned B92 state.

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