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Toward computability of trace distance discord

F Ciccarello[1,4], **T Tufarelli**[2] **and V Giovannetti**[3]

[1] NEST, Istituto Nanoscienze-CNR and Dipartimento di Fisica e Chimica, Università degli Studi di Palermo, Via Archirafi 36, I-90123 Palermo, Italy
[2] QOLS, Blackett Laboratory, Imperial College London, London SW7 2BW, UK
[3] NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, Piazza dei Cavalieri 7, I-56126 Pisa, Italy
E-mail: francesco.ciccarello@unipa.it

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Abstract

It is known that a reliable geometric quantifier of discord-like correlations can be built by employing the so-called trace distance, which is used to measure how far the state under investigation is from the closest 'classical-quantum' state. To date, the explicit calculation of this indicator for two qubits has only been accomplished for states where the reduced density matrix of the measured party is maximally mixed, a class that includes Bell-diagonal states. Here, we first reduce the required optimization for a general two-qubit state to the minimization of an explicit two-variable function. Using this framework, we show that the minimum can be analytically worked out in a number of relevant cases, including quantum-classical and X states. This provides an explicit and compact expression for the trace distance discord of an arbitrary state belonging to either of these important classes of density matrices.

1. Introduction

The issue that the quantum correlations (QCs) of a composite state are not entirely captured by entanglement (as formerly believed) has recently emerged as a topical subject, calling for the introduction of new paradigms. Despite early evidence of this problem, which was provided over a decade ago [2], an impressive burst of attention to this matter has developed only in the last few

[4] Author to whom any correspondence should be addressed.

years [1], as particularly witnessed by very recent experimental works (see e.g. [3, 4]). In this paper, we focus on those correlations that are associated to the notion of *quantum discord* [2]. Following the introduction of this concept, a variety of different measures of QCs have been put forward (see [1] for a comprehensive review). A major reason behind such a proliferation of QCs indicators stems from the typical difficulty of defining a reliable measure that is easily computable. For instance, no general closed formula of quantum discord is known (with strong indications that this is an unsolvable problem [6]), even for a pair of two-dimensional systems or 'qubits' [5]; namely, the simplest composite quantum system. Unfortunately, the demand for computability typically comes at the cost of ending up with quantities that fail to be *bona fide* measures. In this respect, the most paradigmatic instance is embodied by the so called *geometric discord* (GD) [7] which, while being effortlessly computable (and in some cases able to provide useful information), may entail unphysical predictions. It can indeed grow under local operations on the unmeasured party [8], an effect which a physically reliable (bona fide) indicator (e.g. quantum discord) is required not to exhibit. Following an approach frequently adopted for other QCs measures, the one-sided GD is defined as the distance between the state under study and the set of classical-quantum states. The latter class features zero quantum discord with respect to the measured party, say subsystem A, which entails the existence of at least one set of local projective measurements on A leaving the state unperturbed [2, 9]. While the above definition in terms of a distance is clear and intuitive, it requires the use of a metric in the Hilbert space. The GD employs the Hilbert–Schmidt distance, which is defined in terms of the Schatten two-norm. Such a distance is well-known not to fulfil the property of being contractive under trace-preserving quantum channels [10, 11], which is indeed the reason behind the aforementioned drawback of GD [12][5]. This naturally leads to a redefinition of the GD in terms of a metric that obeys the contractivity property. One such metric is the *trace distance* [5, 13], which employs the Schatten one-norm (or trace norm for brevity). In the remainder of this paper, we refer to the QCs geometric measure resulting from this specific choice as *trace distance discord* (TDD).

Although investigations are still in the early stages [14–18], TDD appears to enjoy attractive features, which makes it a physically meaningful measure. Besides the discussed contractivity property, the trace distance is invariant under unitary transformations. More importantly, it is in one-to-one correspondence with *one-shot state distinguishability* [19]; that is, the maximum probability to distinguish between two states through a single measurement. This operational interpretation provides evidence that the trace distance works as an accurate 'meter' in the space of quantum states which, importantly, has a clear physical meaning. Another appealing advantage of TDD lies in its connection with entanglement. Indeed, it was recently suggested to define the full amount of discord-like correlations in a system S as the minimum entanglement between S and the measurement apparatus created in a local measurement (see [20–22] and references therein). This way, a given entanglement measure [23] identifies a corresponding QCs indicator. Remarkably, it turns out that the latter always exceeds the entanglement between the subparts of S when this is quantified via the same entanglement measure. This rigorously formalizes the idea that a composite state can feature QCs that cannot be ascribed to entanglement. In this framework, it can be shown [16] that the

[5] There is an *ad hoc* alternative strategy to overcome some of the pathologies of GD by rescaling this in terms of the state purity as shown in [12]. Although this results in a more reliable QCs quantifier, it is still not sufficient to cure the lack of contractivity of GD.

entanglement counterpart of TDD is *negativity* [24], the latter being a well-known—in general easily computable—entanglement monotone[6].

In spite of all these interesting features, the easiness of computation of TDD in actual problems is yet to be assessed. To date, the only class of states for which a closed analytical expression has been worked out are the Bell-diagonal (BD) two-qubit states or, more generally, states that appear maximally mixed to the measured party [16, 17]. Although the proof of this formula is non-trivial [16], this does not clarify whether or not, besides its reliability, TDD also brings about computability advantages. Owing to the high symmetry and reduced number of parameters of BD states, most if not all of the bona fide QCs measures proposed so far can be analytically calculated for this specific class [26].

In this paper, we take a step forward and set up the problem of the actual computation of two-qubit TDD on a new basis. We first develop a theoretical framework that reduces this task to the equivalent minimization of a two-variable explicit function, which parametrically depends on the Bloch vectors of the marginals and the singular values of the correlation matrix. Next, after re-deriving the value of TDD for a class of density matrices that includes BD states, we discuss two further relevant cases in which the minimization problem can be analytically solved. One is a case where the correlation matrix has one non-zero singular eigenvalue, a subset of which is given by the *quantum-classical* states (unlike classical-quantum states these feature non-classical correlations with respect to party A). The other case is given by the family of X *states* [25], which include BD states as special cases. While these are arguably among the most studied classes of two-qubit density matrices [1], the calculation of their QCs through bona fide measures is in general a demanding task. To the best of our knowledge, no closed expression for an arbitrary quantum-classical state is known to date with the exception of [27] where an ad hoc measure exclusively devised for this specific class of states was presented. In a general case, one such state depends on four independent parameters and features quite low symmetry. For instance, in [27, 28] closed expressions for a fidelity-based measure [29] and the quantum discord, respectively, could be worked out only for high-symmetry two-parameter subsets of this family.

Even more involved is the calculation of QCs in the case of X states; a class which depends on five independent parameters. Regarding quantum discord, an algorithm has been put forward by Ali *et al* [30]. However, some later counterexamples of X states for which such algorithm fails have been highlighted [31] (see also [1]).

The present paper is organized as follows. In section 2, we present our method for tackling and simplifying the calculation of TDD for an arbitrary two-qubit state. This is demonstrably reduced to the minimization of an explicit two-variable function. In section 3, we apply the theory to the case of Bell states and that of density matrices having correlation matrix with uniform spectrum. In section 4, we show that the minimum can be analytically found in a closed form whenever the correlation matrix of the composite state features only one non-zero singular value. As an application of this finding, in section 4.1 we compute the TDD of the most general quantum-classical state. As a further case where the minimization in section 2 can be performed explicitly, in section 5 we tackle the important class of X states and work out the TDD for an arbitrary element of this. In section 6, we illustrate an application of our

[6] In [16], such a counterpart is termed *partial negativity of quantumness*. Rigorously speaking, if the TDD is defined as the trace distance from the closest classical state then it coincides with the negativity of quantumness when the measured party is a qubit. This is sufficient for our goals since we will deal with two-qubit states throughout.

findings to a paradigmatic physical problem (i.e. propagation of QCs across a spin chain), where the analytical calculation of quantum discord [2], although possible, results in uninformative formulae. We show that, while the time behavior of TDD exhibits the same qualitative features as the quantum discord, its analytical expression is quite simple. We finally draw our conclusions in section 7. A few technical details are presented in the appendix.

2. One-sided trace distance discord for two-qubit states: general case

The one-sided TDD $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ from A to B of a bipartite quantum state ρ_{AB} is defined as the minimal (trace norm) distance between such a state and the set $\mathcal{CQ}$ of *classical-quantum* density matrices which exhibit zero quantum discord with respect to local measurements on A; that is, states which admit an unraveling of the form

$$\rho_{AB}^{(\rightarrow)} = \sum_j |\alpha_j\rangle_A\langle\alpha_j| \otimes \varrho_B(j) \tag{1}$$

with $|\alpha_j\rangle_A$ being orthonormal vectors of A and $\varrho_B(j)$ being positive (not necessarily normalized) operators of B. Specifically, if $\|\Theta\|_1 = \mathrm{Tr}[\sqrt{\Theta^\dagger\Theta}]$ denotes the trace norm (or Schatten one-norm) of a generic operator Θ then

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{1}{2}\min_{\{\rho_{AB}^{(\rightarrow)}\}} \|\rho_{AB} - \rho_{AB}^{(\rightarrow)}\|_1 \tag{2}$$

the $1/2$ factor ensuring that $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ takes values between 0 and 1 (an analogous definition applies for the one-sided TDD from B to A, $\mathcal{D}^{(\leftarrow)}(\rho_{AB})$). The quantity in equation (2) fulfils several requirements that make it fit for describing non-classical correlations of the discord type [16]. In particular, from the properties of the trace distance [5] it follows that $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$[7]

(i) is zero if and only if ρ_{AB} is one of the classical-quantum density matrices (1);

(ii) is invariant under the action of an arbitrary unitary operation $U_A \otimes V_B$ that acts locally on A and B; that is,

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) \equiv \mathcal{D}^{(\rightarrow)}(U_A \otimes V_B \rho_{AB} U_A^\dagger \otimes V_B^\dagger); \tag{3}$$

(iii) is monotonically decreasing under completely positive and trace preserving maps on B; and

(iv) is an entanglement monotone when ρ_{AB} is pure.

Furthermore, in a special case in which A is a qubit, equation (2) can be expressed as [16]

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{1}{2}\min_{\{\Pi_A\}} \|\rho_{AB} - (\Pi_A \otimes \mathbb{I}_B)(\rho_{AB})\|_1, \tag{4}$$

where the minimization is now performed with respect to all possible completely depolarizing channels Π_A on A associated with projective measurements over an orthonormal basis; that is,

$$\Pi_A(\cdots) = P_A \ldots P_A + Q_A \ldots Q_A \tag{5}$$

[7] We stress that these properties should not be regarded as mere mathematical features. On the contrary, they embody the requirement that the used measure fulfil some fundamental physical constraints.

with $P_A \equiv |\Psi\rangle_A\langle\Psi|$ and $Q_A = \mathbb{I}_A - P_A$ being rank-one projectors ($|\Psi\rangle$ is a generic one-qubit *pure* state).

In what follows, we will focus on a case where *both* A and B are qubits. Accordingly, we parameterize the state ρ_{AB} in terms of the Pauli matrices $\vec{\sigma}_{A(B)} = \{\sigma_{A(B)1}, \sigma_{A(B)2}, \sigma_{A(B)3}\} \equiv \{\sigma_{A(B)x}, \sigma_{A(B)y}, \sigma_{A(B)z}\}$, i.e.

$$\rho_{AB} = \frac{1}{4}\left(\mathbb{I}_A \otimes \mathbb{I}_B + \vec{x}_A \cdot \vec{\sigma}_A \otimes \mathbb{I}_B + \mathbb{I}_A \otimes \vec{x}_B \cdot \vec{\sigma}_B + \sum_{i,j=1}^{3} \Gamma_{ij}\sigma_{Ai} \otimes \sigma_{Bj}\right), \tag{6}$$

where

$$\vec{x}_{A(B)} = \mathrm{Tr}\,[\rho_{AB}\vec{\sigma}_{A(B)}] \tag{7}$$

is the Bloch vector corresponding to the reduced density matrix $\rho_{A(B)}$ describing the state of $A(B)$, while Γ is the 3×3 real correlation matrix given by

$$\Gamma_{ij} = \mathrm{Tr}\,[\rho_{AB}(\sigma_{Ai} \otimes \sigma_{Bj})]. \tag{8}$$

Similarly, without loss of generality, we express the orthogonal projectors P_A and Q_A of equation (5) as

$$P_A = \tfrac{1}{2}(\mathbb{I}_A + \hat{e} \cdot \vec{\sigma}_A), \quad Q_A = \tfrac{1}{2}(\mathbb{I}_A - \hat{e} \cdot \vec{\sigma}_A) \tag{9}$$

with $\hat{e}$ being the three-dimensional (real) unit vector associated with the pure state $|\Psi\rangle_A$ in the Bloch sphere. Using this and observing that $\Pi_A(\mathbb{I}_A) = \mathbb{I}_A$, and $\Pi_A(\vec{v} \cdot \vec{\sigma}_A) = (\hat{e} \cdot \vec{v})\,(\hat{e} \cdot \vec{\sigma}_A)$, equation (4) can be arranged as

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \tfrac{1}{8}\min_{\hat{e}} \|M(\hat{e})\|_1, \tag{10}$$

where the minimization is performed over the unit vector $\hat{e}$ and $M(\hat{e})$ is a 4×4 matrix which admits the representation

$$M(\hat{e}) = \left[(\vec{x}_A - (\hat{e} \cdot \vec{x}_A)\hat{e}) \cdot \vec{\sigma}_A\right] \otimes \mathbb{I}_B + \sum_{ij} \Gamma_{ij}\ (\hat{x}_i - e_i\hat{e}) \cdot \vec{\sigma}_A \otimes \sigma_{Bj}. \tag{11}$$

Here, $\hat{x}_i$ is the ith Cartesian unit vector and $e_i = \hat{x}_i \cdot \hat{e}$ the ith component of $\hat{e}$ (note that $\sigma_{Ai} = \hat{x}_i \cdot \vec{\sigma}_A$). The second term in equation (11) can be further simplified by transforming Γ into a diagonal form via its singular value decomposition [32]. More precisely, by exploiting the fact that Γ is real we can express it as

$$\Gamma = O^{\top}\begin{bmatrix}\gamma_1 & 0 & 0\\ 0 & \gamma_2 & 0\\ 0 & 0 & \gamma_3\end{bmatrix}\Omega, \tag{12}$$

where O and Ω are real orthogonal matrices of $SO(3)$ while $\{\gamma_i\}$ are real (not necessarily non-negative) quantities whose moduli correspond to the singular eigenvalues of Γ.[8] We can then

[8] Dealing with O, Ω that are elements of $SO(3)$—instead of its subset $O(3)$—is fundamental to ensure that the orthonormal sets of vectors pin equation (13) are properly right-hand oriented. This possibility comes explicitly from the fact that we allow for negative γ_k's in equation (12). Indeed, the standard singular value decomposition would yield $\Gamma = \tilde{O}^{\top}\mathrm{diag}\,(|\gamma_1|, |\gamma_2|, |\gamma_3|)\tilde{\Omega}$ with $\tilde{O}, \tilde{\Omega}$ elements of $O(3)$ [32]. The last identity can then be put in the form of equation (12) by observing that there exist T, T' diagonal elements of $O(3)$ representing spatial inversions and $O, \Omega \in SO(3)$ which allow us to write $\tilde{O} = TO$ and $\tilde{\Omega} = T'\Omega$. Accordingly, we obtain $\Gamma = O^{\top}\mathrm{diag}T(|\gamma_1|, |\gamma_2|, |\gamma_3|)T'\Omega$, which coincides with equation (12) once one observes that by construction the diagonal entries of T and T' can only be equal to either 1 or -1.

define the two sets of vectors

$$\hat{w}_k = \sum_{j=1}^{3} O_{kj}\hat{x}_j, \quad \hat{\upsilon}_k = \sum_{j=1}^{3} \Omega_{kj}\hat{x}_j \tag{13}$$

for $k = 1, 2, 3$. As $O, \Omega \in SO(3)$, by construction $\{\hat{w}_k\}$ is an orthonormal (right-hand oriented) set of real vectors and so is $\{\hat{\upsilon}_k\}$ (each is indeed a rotation of the Cartesian unit vectors $\{\hat{x}_j\}$). Using the above, we can arrange equation (11) as

$$M(\hat{e}) = (\vec{x}_{A\perp}\cdot\vec{\sigma}_A)\otimes\mathbb{I}_B + \sum_{k=1}^{3}\gamma_k\,(\vec{w}_{k\perp}\cdot\vec{\sigma}_A)\otimes\left(\hat{\upsilon}_k\cdot\vec{\sigma}_B\right), \tag{14}$$

where, for compactness of notation, we introduce the vectors

$$\vec{x}_{A\perp} = \vec{x}_A - (\hat{e}\cdot\vec{x}_A)\hat{e}, \quad \vec{w}_{k\perp} = \hat{w}_k - (\hat{e}\cdot\hat{w}_k)\hat{e} \tag{15}$$

to represent the orthogonal component of $\vec{x}_A$ and $\hat{w}_k$ with respect to $\hat{e}$.

Note that $\{\hat{\upsilon}_k\cdot\vec{\sigma}_B\}$ describes the transformed set of Pauli matrices under a local rotation on B. This set clearly also fulfils all the properties of Pauli matrices. One can, therefore, redefine the B's Pauli matrices as $\{\hat{\upsilon}_k\cdot\vec{\sigma}_B\}\to\sigma_{Bk}$, which amounts to applying a local unitary on B. Then let $M'(\hat{e})$ be the transformed operator obtained from $M(\hat{e})$ under such rotation; that is,

$$M'(\hat{e}) = (\vec{x}_{A\perp}\cdot\vec{\sigma}_A)\otimes\mathbb{I}_B + \sum_{k=1}^{3}\gamma_k\,(\vec{w}_{k\perp}\cdot\vec{\sigma}_A)\otimes\sigma_{Bk}. \tag{16}$$

Since the trace norm is invariant under any local unitary, we have

$$\|M(\hat{e})\|_1 = \|M'(\hat{e})\|_1 \tag{17}$$

which is in line with the invariance property (ii) of $\mathcal{D}^{(\to)}(\rho_{AB})$ (indeed $M'(\hat{e})$ is the operator (11) associated to the state ρ'_{AB} obtained from ρ_{AB} via a local unitary rotation associated to the transformation $\{\hat{\upsilon}_k\cdot\vec{\sigma}_B\}\to\sigma_{Bk}$). The trace norm of $M'(\hat{e})$ can now be computed by diagonalizing the operator $M'(\hat{e})^\dagger M'(\hat{e})$. For this purpose, we recall that, given two arbitrary vectors $\{\vec{x},\,\vec{y}\}$, the Pauli matrices fulfil the following commutation and anti-commutation relations:

$$[\vec{x}\cdot\vec{\sigma}_A,\,\vec{y}\cdot\vec{\sigma}_A] = 2\mathrm{i}\,(\vec{x}\wedge\vec{y})\cdot\vec{\sigma}_A, \tag{18}$$

$$\{\vec{x}\cdot\vec{\sigma}_A,\;\vec{y}\cdot\vec{\sigma}_A\} = 2\,(\vec{x}\cdot\vec{y}) \tag{19}$$

as well as the identities $\sigma_{A1}\sigma_{A2} = \mathrm{i}\sigma_{A3}$, $\sigma_{A2}\sigma_{A1} = -\mathrm{i}\sigma_{A3}$ and the analogous identities obtained through cyclic permutations (in the above expression '$\wedge$' indicates the cross product). Using these, we straightforwardly end up with

$$M'(\hat{e})^\dagger M'(\hat{e}) = \left(Q + x_{A\perp}^2\right)\mathbb{I}_{AB} + \Delta + 2\,\mathbb{I}_A\otimes\vec{\chi}\cdot\vec{\sigma}_B, \tag{20}$$

where $x_{A\perp} = |\vec{x}_{A\perp}|$ (throughout, $x = |\vec{x}\,|$ for any vector $\vec{x}$), $\vec{\chi}$ is a tridimensional real vector of components

$$\chi_k = \gamma_k\,\vec{w}_{k\perp}\cdot\vec{x}_{A\perp}, \tag{21}$$

while Q is a positive quantity defined as

$$Q = \sum_{k=1}^{3}\gamma_k^2\,|\vec{w}_{k\perp}|^2 \tag{22}$$

and, finally, Δ is the operator

$$\begin{aligned}\Delta &= \sum_{j\neq k}\gamma_j\gamma_k\left[(\vec{w}_{j\perp}\cdot\vec{\sigma}_A)(\vec{w}_{k\perp}\cdot\vec{\sigma}_A)\otimes\sigma_{Bj}\sigma_{Bk}\right]\\ &= -2\gamma_1\gamma_2\,(\vec{w}_{1\perp}\wedge\vec{w}_{2\perp})\cdot\vec{\sigma}_A\otimes\sigma_{B3}-2\gamma_2\gamma_3\,(\vec{w}_{2\perp}\wedge\vec{w}_{3\perp})\cdot\vec{\sigma}_A\otimes\sigma_{B1}\\ &\quad -2\gamma_3\gamma_1\,(\vec{w}_{3\perp}\wedge\vec{w}_{1\perp})\cdot\vec{\sigma}_A\otimes\sigma_{B2}.\end{aligned}\tag{23}$$

This expression can be simplified by observing that, since the $\vec{w}_{k\perp}$'s are vectors orthogonal to $\hat{e}$ (see equation (15)), their mutual cross products must be collinear with the latter. Indeed, by introducing the spherical coordinates $\{\theta,\phi\}$ that specify $\hat{e}$ in the reference frame defined by $\{\hat{w}_k\}$, we have

$$\begin{aligned}(\vec{w}_{1\perp}\wedge\vec{w}_{2\perp}) &= (\hat{w}_3\cdot\hat{e})\,\hat{e}=\cos\theta\,\hat{e},\\ (\vec{w}_{2\perp}\wedge\vec{w}_{3\perp}) &= (\hat{w}_1\cdot\hat{e})\,\hat{e}=\sin\theta\cos\phi\,\hat{e},\\ (\vec{w}_{3\perp}\wedge\vec{w}_{1\perp}) &= (\hat{w}_2\cdot\hat{e})\,\hat{e}=\sin\theta\sin\phi\,\hat{e}.\end{aligned}\tag{24}$$

By substituting these identities in equation (23), the operator Δ can remarkably be arranged in terms of a simple tensor product as

$$\Delta=-2\,(\hat{e}\cdot\vec{\sigma}_A)\otimes(\vec{g}\cdot\vec{\sigma}_B),\tag{25}$$

where $\vec{g}$ is the vector

$$\vec{g}=(\gamma_2\gamma_3\sin\theta\cos\phi,\,\gamma_3\gamma_1\sin\theta\sin\phi,\,\gamma_1\gamma_2\cos\theta),\tag{26}$$

which is orthogonal to $\vec{\chi}$.[9] Next, observe that the operator $\hat{e}\cdot\vec{\sigma}_A$ of equation (25) is Hermitian with eigenvalues 1 and -1. Therefore, if $\{|0\rangle_A,|1\rangle_A\}$ are its eigenvectors, then we can write $\hat{e}\cdot\vec{\sigma}_A=|0\rangle_A\langle 0|-|1\rangle_A\langle 1|$. By plugging this and $\mathbb{I}_A=|0\rangle_A\langle 0|+|1\rangle_A\langle 1|$ into equation (20), this can be arranged as

$$M'(\hat{e})^\dagger M'(\hat{e})=(Q+x_{A\perp}^2)\mathbb{I}_{AB}+2\left[|0\rangle_A\langle 0|\otimes(\vec{\chi}-\vec{g})\cdot\vec{\sigma}_B+|1\rangle_A\langle 1|\otimes(\vec{\chi}+\vec{g})\cdot\vec{\sigma}_B\right],$$

which can now be put in diagonal form. Indeed, due to the aforementioned spectrum of $\vec{x}\cdot\vec{\sigma}$, it has eigenvalues $\lambda=Q+x_{A\perp}^2\pm 2\sqrt{\chi^2+g^2}$, each twofold degenerate (see footnote 9). Therefore, through equation (17), we end up with

$$\|M(\hat{e})\|_1=2\left(\sqrt{a+\sqrt{b}}+\sqrt{a-\sqrt{b}}\right),\tag{27}$$

where

$$a=a(\hat{e})=Q+x_{A\perp}^2=Q+x_A^2-(\vec{x}_A\cdot\hat{e})^2,\tag{28}$$

$$b=b(\hat{e})=4\left(\chi^2+g^2\right).\tag{29}$$

Note that Q, $x_{A\perp}$, χ and g are all functions of $\hat{e}$ (cf equations (21), (22) and (26)). As $\|M(\hat{e})\|_1$ is a positive-definite function, finding its minimum is equivalent to searching for the minimum of its square $\|M(\hat{e})\|_1^2$. Thereby

$$\min_{\hat{e}}\|M(\hat{e})\|_1=\sqrt{\min_{\hat{e}}\|M(\hat{e})\|_1^2}=2\sqrt{2\left[\min_{\hat{e}}h(\hat{e})\right]},\tag{30}$$

[9] The orthogonality between $\vec{g}$ of equation (26) and $\vec{\chi}$ of equation (21) follows from the fact that when computing $\vec{\chi}\cdot\vec{g}$ the γ's can be factored out of the sum to give $\vec{\chi}\cdot\vec{g}=\gamma_1\gamma_2\gamma_3\left[\vec{x}_A-\hat{e}(\hat{e}\cdot\vec{x}_A)\right]\cdot\hat{e}=0$. Exploiting this identity, one can then write $|\vec{\chi}\pm\vec{g}|\equiv\sqrt{\chi^2+g^2}$.

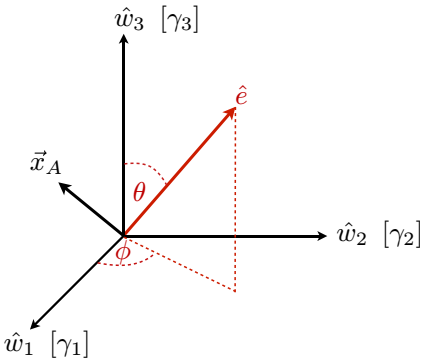

Figure 1. Schematics of the minimization procedure for calculating the TDD $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ of a two-qubit state ρ_{AB}. The reference frame in which this is carried out is defined by the orthonormal set of three vectors $\{\hat{w}_k\}$, where each $\hat{w}_k$ is associated with a real singular eigenvalue γ_k of the correlation matrix (see equations (8), (12) and (13)). This frame identifies a representation for the local Bloch vector $\vec{x}_A$ (defined in equation (7)). All these quantities are drawn using solid black lines to highlight that, for a given density matrix ρ_{AB}, they are fixed. Instead, the unit vector $\hat{e}$ (red line) represents the direction along which a projective measurement on A is performed. In the optimization procedure, $\hat{e}$ is varied until function h in equation (31) reaches its global minimum according to equation (32).

where the function $h(\hat{e})$ is defined as

$$h(\hat{e}) = a(\hat{e}) + \sqrt{a^2(\hat{e}) - b(\hat{e})}. \tag{31}$$

In conclusion, in the light of equations (10), (27) and (30)

$$\begin{aligned}\mathcal{D}^{(\rightarrow)}(\rho_{AB}) &= \frac{1}{4}\min_{\hat{e}}\left[\sqrt{a+\sqrt{b}}+\sqrt{a-\sqrt{b}}\right] \\ &= \frac{1}{4}\sqrt{2\left[\min_{\hat{e}} h\right]}.\end{aligned} \tag{32}$$

We have thus expressed our trace-norm-based measure of QCs of an arbitrary state ρ_{AB} as the minimum of an *explicit* function of the two angles $\{\theta, \phi\}$ $(0 \leqslant \theta \leqslant \pi,\ 0 \leqslant \phi \leqslant 2\pi)$. Equation (32) is the first main finding of this paper. For clarity, all quantities involved in the minimization problem under investigation are pictorially represented in figure 1.

3. Bell diagonal states and states with homogeneous singular values

The optimization in equation (32) simplifies when the state possesses certain symmetries. In particular, by ordering the singular eigenvalues of Γ as (this convention is adopted only in the present section)

$$|\gamma_1| \geqslant |\gamma_2| \geqslant |\gamma_3|, \tag{33}$$

one can show that

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{|\gamma_2|}{2}, \tag{34}$$

at least for two classes of states ρ_{AB}, which we label as 'A' and 'B', respectively. These are defined as

$$\begin{aligned}&\text{Class A : arbitrary } \{\gamma_k\} \text{ but } \vec{x}_A = 0.\\ &\text{Class B : arbitrary } \vec{x}_A \text{ but } \{\gamma_k\} \text{ with the equal moduli, i.e.}\\ &|\gamma_k| = \gamma \qquad \forall k = 1, 2, 3.\end{aligned} \tag{35}$$

We develop the proof in the following two subsections.

3.1. Bell diagonal states

States of class A, which include Bell diagonal states, are characterized by the property that the reduced density matrix of subsystem A is maximally mixed. For these, equation (34) was proven in [16, 17] using an independent approach. Here, we present an alternative (possibly simpler) derivation based on equation (32). We point out that these states form a special subset of X states, which we will study in full detail in section 5. Here, our goal is to present a straightforward application of our method for calculating the TDD, which was developed in the previous section.

To begin with, we observe that if $\vec{x}_A = 0$ then the vector $\vec{\chi}$ in equation (21) vanishes (i.e. $\vec{\chi} = 0$) while the function a in equation (28) coincides with Q in equation (22). Thereby, the function h in equation (31), which we have to minimize over $\hat{e}$ according to equation (32), becomes

$$h = Q + \sqrt{H} \quad \text{with} \quad H = Q^2 - 4\,g^2. \tag{36}$$

Expressing now Q in terms of θ and ϕ, and due to the ordering in equation (33), it turns out that

$$\begin{aligned}Q(\theta,\phi) &= \gamma_1^2(1-\cos^2\phi\sin^2\theta) + \gamma_2^2(1-\sin^2\phi\sin^2\theta) + \gamma_3^2(1-\cos^2\theta)\\ &\geqslant Q(\theta=\pi/2,\phi=0) = \gamma_2^2+\gamma_3^2,\end{aligned} \tag{37}$$

namely Q reaches its minimum value for $\theta = \pi/2$ and $\phi = 0$; that is, when $\hat{e}$ points toward $\hat{w}_1$. The same property holds for the function H. Indeed one has

$$\begin{aligned}H(\theta,\phi) &= A(\theta)\ \sin^4\phi + B(\theta)\ \sin^2\phi + C(\theta)\\ &\geqslant H(\theta=\pi/2,\phi=0) = (\gamma_2^2-\gamma_3^2)^2,\end{aligned} \tag{38}$$

where we used

$$A(\theta) = \sin^4\theta\ (\gamma_1^2 - \gamma_2^2)^2 \geqslant A(0) = 0,$$

$$B(\theta) = 2\ \sin^2\theta\ (\gamma_1^2 - \gamma_2^2)[(\gamma_2^2 - \gamma_3^2) + \cos^2\theta\ (\gamma_1^2 - \gamma_3^2)] \geqslant B(0) = 0,$$

$$C(\theta) = (\gamma_2^2-\gamma_3^2)^2 + 2\cos^2\theta(\gamma_2^2+\gamma_3^2)(\gamma_1^2 - \gamma_3^2) + \cos^4\theta(\gamma_1^2-\gamma_3^2)^2 \geqslant C(\theta=\pi/2) \geqslant (\gamma_2^2-\gamma_3^2)^2.$$

Replacing equations (37) and (38) into equation (36) entails $h(\theta,\phi) \geqslant h(\theta=\pi/2,\phi=0) \geqslant 2|\gamma_2|^2$, which through equation (32) yields equation (34).

3.2. States with homogeneous $|\gamma_k|$'s

Class B (see definition given above) includes, for instance, mixtures of the form $\rho_{AB} = p\varrho_A \otimes \mathbb{I}_B/2 + (1-p)|\Psi_-\rangle_{AB}\langle\Psi_-|$ where $p \in [0,1]$, ϱ_A is an arbitrary state of A, and $|\Psi_{AB}\rangle$ is the singlet state $|\Psi_{AB}\rangle = (|01\rangle_{AB} - |10\rangle_{AB})/\sqrt{2}$ (from now on, $\{|0\rangle_{A(B)}, |1\rangle_{A(B)}\}$ denotes an orthonormal basis for A (B)). In this case, $\gamma_k = (1-p)$ for all k while $\vec{x}_A = p\vec{s}_A$ with $\vec{s}_A$ the Bloch vector of ϱ_A; therefore, according to equation (34), this state has a value for TDD given by $(1-p)/2$.

To derive equation (34), we introduce the diagonal matrix $T = \mathrm{diag}\,(t_{11}, t_{22}, t_{33})$ formed by the coefficients t_{11}, t_{22}, t_{33} defined by the identities

$$\gamma_j = t_{jj}\,\gamma \tag{39}$$

(it is clear from (35) that t_{jj} can only take values ± 1). Under this condition, from equations (21), (22) and (26) it then follows

$$\begin{aligned} Q &= 2\gamma^2, \\ \vec{g} &= \xi\,\gamma^2\,T\,\hat{e} \Longrightarrow |\vec{g}|^2 = \gamma^4, \\ \vec{\chi} &= \gamma\,T\,\vec{x}_{A,\perp} \Longrightarrow |\vec{\chi}|^2 = \gamma^2|\vec{x}_{A,\perp}|^2, \end{aligned} \tag{40}$$

where ξ takes value either 1 or -1 depending on the explicit form of the mapping (39). Replacing this into equations (28), (29) and (31) we end up with

$$h = 2\gamma^2 + 2|\vec{x}_{A,\perp}|^2, \tag{41}$$

which depends upon $\hat{e}$ through $|\vec{x}_{A,\perp}|^2$ only. The minimum is then achieved when $|\vec{x}_{A,\perp}|$ vanishes, which clearly occurs by taking $\hat{e}$ along the direction of $\vec{x}_A$ (recall equation (15)). Thus,

$$\min_{\hat{e}} h = 2\gamma^2 \tag{42}$$

which when replaced into equation (32) gives equation (34), as anticipated.

4. Correlation matrix with a single non-zero singular eigenvalue

This class of states is important since quantum-classical states fall within it, as we show later. It is defined by (see equation (12)) $\gamma_2 = \gamma_3 = 0$ while $\gamma_1 = \gamma$ and $\vec{x}_A$ are arbitrary (the only constraint is that the resulting ρ_{AB} must be a properly defined density matrix). We show below that the TDD of one such state is given by

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{|\vec{\gamma}_1 \wedge \vec{x}_A|}{2} \min\left\{\frac{1}{|\vec{\gamma}_1 \pm \vec{x}_A|}\right\}, \tag{43}$$

where $\vec{\gamma}_1 = |\gamma_1|\hat{w}_1$, $\hat{w}_1$ being the first element of the set $\{\hat{w}_k\}$ defined in equation (13). Equation (43) is another main finding of this work.

To begin with, we observe that due to $\gamma_2 = \gamma_3 = 0$ we are free to choose the direction of the Cartesian axes $\hat{w}_2$ and $\hat{w}_3$ ($\hat{w}_2 \perp \hat{w}_3$) on the plane orthogonal to $\hat{w}_1$. We, thus, take $\hat{w}_2$ as lying on the plane formed by $\hat{w}_1$ and $\vec{x}_A$. Hence, we can write $\vec{x}_A = \tilde{x}_{A1}\hat{w}_1 + \tilde{x}_{A2}\hat{w}_2$, where $\tilde{x}_{A1}$ and $\tilde{x}_{A2}$ are the components of $\vec{x}_A$ in a reference frame defined by $\{\hat{w}_k\}$. Accordingly,

$$\tilde{x}_{A1} = \hat{x}_A \cdot \hat{w}_1 = x_A \cos\alpha, \quad \tilde{x}_{A2} = \hat{x}_A \cdot \hat{w}_2 = x_A \sin\alpha \tag{44}$$

with α being the angle between $\vec{x}_A$ and $\hat{w}_1$ while $x_A = \sqrt{\tilde{x}_{A1}^2 + \tilde{x}_{A2}^2}$. With the help of equations (21), (22) and (26), in the present case a and b (cf equations (28) and (29)) read

$$a = \gamma^2 + x_A^2 - [\gamma^2 \tilde{e}_1^2 + (\hat{e}\cdot\vec{x}_A)^2], \quad b = 4\gamma^2[\tilde{x}_{A1} - \tilde{e}_1(\hat{e}\cdot\vec{x}_A)]^2, \tag{45}$$

where $\tilde{e}_1 = \hat{e}\cdot\hat{w}_1$. Then we can write

$$a \pm \sqrt{b} = (\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2 - \left[\gamma\tilde{e}_1 \pm (\hat{e}\cdot\vec{x}_A)\right]^2. \tag{46}$$

It turns out that *both* $a+\sqrt{b}$ *and* $a-\sqrt{b}$ decrease when the component of $\hat{e}$ on the plane formed by $\hat{w}_1$ and $\vec{x}_A$ (i.e. the $\hat{w}_1 - \hat{w}_2$ plane) grows. To see this, we decompose $\hat{e}$ as $\hat{e} = \vec{\varepsilon} + \vec{\varepsilon}_\perp$, where $\vec{\varepsilon} = \tilde{e}_1\hat{w}_1 + \tilde{e}_2\hat{w}_2$ is the component of $\hat{e}$ on the $\hat{w}_1 - \hat{w}_2$ plane, while $\vec{\varepsilon}_\perp = \tilde{e}_3\hat{w}_3$ is the one orthogonal to it. With these definitions, in equation (46) we can evidently replace $\hat{e}$ with $\vec{\varepsilon}$ (we remind that $\tilde{x}_{A3} = 0$). Now, it should be evident that the last term of equation (46) can be written as $-\left[\gamma\tilde{e}_1 \pm (\hat{e}\cdot\vec{x}_A)\right]^2 = -|\varepsilon|^2[f_\pm(\phi,\alpha)]^2$, where $f_\pm(\phi,\alpha) = \gamma\cos\phi \pm x_A\cos(\phi-\alpha)$ is a function of ϕ (i.e. the azimuthal angle of $\hat{e}$) and the aforementioned α. Clearly, for given ϕ, the minimum of $a \pm \sqrt{b}$ is achieved when $|\vec{\varepsilon}|$ is maximum; that is, for $\vec{\varepsilon} \equiv \hat{e}$ or equivalently $\theta = \pi/2$. Thus, due to equation (27), in equation (32) we can safely restrict the minimization over $\hat{e} = (\theta,\phi)$ to the set $\hat{e} = (\pi/2,\phi)$. To summarize, we need to calculate

$$\min_\phi \left[\|M(\hat{e})\|_1 \Big|_{\theta=\frac{\pi}{2}} \right] = 2\sum_{\eta=\pm} \sqrt{(\gamma + \eta\tilde{x}_{A1})^2 + \tilde{x}_{A2}^2 - f_\eta(\phi,\alpha)^2}. \tag{47}$$

Through a few straightforward steps (see appendix A), $\|M(\hat{e})\|_1$ can be arranged as (we henceforth omit to specify $\theta = \pi/2$)

$$\|M(\hat{e})\|_1 = 2\sum_{\eta=\pm} |x_A\sin(\phi-\alpha) + \eta\gamma\sin\phi|\,. \tag{48}$$

By exploiting the positiveness of $\|M(\hat{e})\|_1$, and the identity $(|y+z|+|y-z|)^2 = 4\max\{y^2, z^2\}$, where y and z are any two real numbers, equation (48) can be converted into

$$\begin{aligned}\|M(\hat{e})\|_1 &= 4\max\{|x_A\sin(\phi-\alpha)|\,, |\gamma\sin\phi|\} \\ &= 4\sqrt{x_A^2+\gamma^2}\ \max\{|\sin\beta\sin(\phi-\alpha)|, |\cos\beta\sin\phi|\}\,,\end{aligned} \tag{49}$$

where the angle β is defined through the identity

$$\sin\beta = |x_A|/\sqrt{x_A^2+\gamma^2}. \tag{50}$$

Replacing $\|M(\hat{e})\|$ so obtained into equation (10) we can then express the one-sided TDD of our state ρ_{AB} in terms of the following min–max problem:

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{\sqrt{x_A^2+\gamma^2}}{2} \times \min_{\phi\in[0,2\pi]} \max\{|\sin\beta\sin(\phi-\alpha)|, |\cos\beta\sin(\phi)|\} \tag{51}$$

An analytic solution is obtained by observing that the ϕ-dependent functions $f_1(\phi) = |\sin\beta\sin(\phi-\alpha)|$ and $f_2(\phi) = |\cos\beta\sin(\phi)|$ have the same period π and that in the domain $\phi\in[0,\pi]$ exhibit the two crossing points ϕ_{c+} and ϕ_{c-} given by

$$\cot(\phi_{c\pm}) = \cot\alpha \pm \left|\frac{\cot\beta}{\sin\alpha}\right|. \tag{52}$$

By construction, the function equation (49) reaches its minimum either in ϕ_{c+} or in ϕ_{c-}. Therefore,

$$\begin{aligned}\mathcal{D}^{(\rightarrow)}(\rho_{AB}) &= \frac{\sqrt{x_A^2+\gamma^2}}{2}\min\{|\cos\beta\sin(\phi_{c+})|, |\cos\beta\sin(\phi_{c-})|\} \\ &= \frac{|\gamma\tilde{x}_{A2}|}{2}\min\left\{\frac{1}{\sqrt{(\gamma\pm\tilde{x}_{A1})^2+\tilde{x}_{A2}^2}}\right\},\end{aligned} \tag{53}$$

where the latter identity has been obtained through simple algebraic manipulations. To arrange this formula in a form independent of the reference frame, we make use of equations (44) and (50). This finally yields equation (43).

4.1. Quantum-classical states

The result of the previous section can be exploited to provide an analytical closed formula of $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ for the well-known class of quantum-classical states. One such state reads

$$\rho_{AB} = p\,\rho_{0A}\otimes|0\rangle_B\langle 0| + (1-p)\rho_{1A}\otimes|1\rangle_B\langle 1|, \tag{54}$$

where $\rho_{0(1)}$ is an arbitrary single-qubit state with associated Bloch vector $\vec{s}_{0(1)}$; that is, $\rho_{0(1)} = (\mathbb{I}+\vec{s}_{0(1)}\cdot\vec{\sigma})/2$. The state in equation (54) represents a paradigmatic example of a separable state that is still able to feature $A\rightarrow B$ QCs. On the other hand, note that the quantum discord in the opposite direction, $B\rightarrow A$, is zero by construction.

One can assume without loss of generality that $\vec{s}_0 = (0,0,s_0)$ and $\vec{s}_1 = (s_1\sin\varphi, 0, s_1\cos\varphi)$ with $0\leqslant\varphi\leqslant\pi$; that is, the Z-axis of the Bloch sphere is taken along the direction of $\vec{s}_0$ while the Y-axis lies orthogonal to the plane containing both $\vec{s}_0$ and $\vec{s}_1$. Vector $\vec{x}_A$ and matrix Γ are calculated as

$$\vec{x}_A = (\,(1-p)s_1\sin\varphi, 0, ps_0+(1-p)s_1\cos\varphi\,), \tag{55}$$

$$\Gamma = \begin{pmatrix} 0 & 0 & (1-p)s_1\sin\varphi \\ 0 & 0 & 0 \\ 0 & 0 & ps_0+(1-p)s_1\cos\varphi \end{pmatrix}. \tag{56}$$

Γ has only one singular eigenvalue since its singular value decomposition yields $\gamma_2=\gamma_3=0$ and

$$|\gamma_1| = \gamma = \sqrt{p^2s_0^2+(p-1)s_1\,[(p-1)s_1+2ps_0\cos\varphi]}. \tag{57}$$

Such states, therefore, fall exactly in the case studied in the previous section. To apply equation (43), though, we need to calculate the unit vectors $\hat{w}_k$. From the matrix equation (56), they are calculated as

$$\hat{w}_1 = \frac{1}{\Delta_1}((p-1)s_1\sin\varphi, 0, ps_0+(p-1)s_1\cos\varphi), \tag{58}$$

$$\hat{w}_2 = \frac{1}{\Delta_2}\left(\frac{(1-p)s_1\cot\varphi - ps_0\csc\varphi}{(p-1)s_1}, 0, 1\right), \tag{59}$$

$$\hat{w}_3 = (0,1,0), \tag{60}$$

where $\Delta_{1,2}$ are normalization coefficients. In particular, it turns out that Δ_1 coincides with γ in equation (57), i.e. $\Delta_1 = \gamma$. Hence, the vector $\vec{\gamma}_1 = \gamma\,\hat{w}_1$ in equation (43) is given by

$$\vec{\gamma}_1 = (\,(p-1)s_1 \sin\varphi,\, 0,\, ps_0 + (p-1)s_1 \cos\varphi). \tag{61}$$

This, together with equation (55), yields the identities

$$\begin{aligned} |\vec{x}_A \wedge \vec{\gamma}_1| &= 2p(1-p)\, s_0 s_1 \sin\varphi, \\ |\vec{\gamma}_1 + \vec{x}_A| &= 2p\, s_0, \\ |\vec{\gamma}_1 - \vec{x}_A| &= 2(1-p)\, s_1. \end{aligned}$$

Replacing these into equation (43), we end up with

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{\sin\varphi}{2}\, \min\{ps_0,\, (1-p)s_1\}, \tag{62}$$

which represents the TDD of the most general quantum-classical state (equation (54)). This formula has a very clear interpretation in terms of the lengths of the local Bloch vectors on A, s_0, s_1, the angle between them φ and the statistical weights $p, 1-p$. One can see that the maximum value of $\mathcal{D}^{(\rightarrow)}$ is 1/4 and is obtained for $s_0 = s_1 = 1$, $p = 1/2$ and $\varphi = \pi/2$. This corresponds to picking on system A two pure states with orthogonal Bloch vectors; that is, two vectors belonging to mutually unbiased bases. Indeed, for these parameters, equation (54) reduces to $\rho_{AB} = 1/2\,(|0\rangle_A\langle 0| \otimes |0\rangle_B\langle 0| + |+\rangle_A\langle +| \otimes |1\rangle_B\langle 1|)$ (where $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$), which is a paradigmatic example of a separable but quantum-correlated state. The qualitative behavior of $\mathcal{D}$ for $s_0 = s_1$ and $p = 1/2$ is fully in line with that of the quantum discord [28] and for $s_0 = s_1 = 1$ with that of the fidelity-based measure analyzed in [27].

5. *X* states

A two-qubit X state has the X-shaped matrix form

$$\rho_{AB} = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{41}^* \\ 0 & \rho_{22} & \rho_{32}^* & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix} \tag{63}$$

subject to the constraints $\sum_{i=1}^4 \rho_{ii} = 1$, $\rho_{11}\rho_{44} \geqslant |\rho_{14}|^2$ and $\rho_{22}\rho_{33} \geqslant |\rho_{23}|^2$. Here, we have referred to the computational basis $\{|00\rangle_{AB}, |01\rangle_{AB}, |10\rangle_{AB}, |11\rangle_{AB}\}$. Without loss of generality, off-diagonal entries ρ_{32} and ρ_{41} can be taken as positive; that is, $\rho_{32} \geqslant 0$ and $\rho_{41} \geqslant 0$[10]. It is straightforward to check that for such states $x_{A,1} = x_{A,2} = 0$, $x_{A3} = 2(\rho_{11} + \rho_{22}) - 1$ (that is, $\vec{x}_A$ lies along the $\hat{x}_3$-axis) while the correlation matrix already has a diagonal form since $\Gamma = \mathrm{diag}\,\{\gamma_1, \gamma_2, \gamma_3\}$ with

$$\gamma_1 = 2(\rho_{32} + \rho_{41}), \quad \gamma_2 = 2(\rho_{32} - \rho_{41}), \quad \gamma_3 = 1 - 2(\rho_{22} + \rho_{33}). \tag{64}$$

Hence, in the present case $\hat{w}_k = \hat{x}_k$ for $k = 1, 2, 3$ (see equation (13)). We, therefore, have to deal with the four parameters x_{A3} and $\{\gamma_k\}$. Note that the only hierarchical relation that always holds is $|\gamma_1| \geqslant |\gamma_2|$ (see equation (64)).

[10] One can indeed get rid of phase factors $e^{i \arg \rho_{32}}$ and $e^{i \arg \rho_{41}}$ through local unitaries, which does not affect $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$.

In what follows, we will prove that the TDD of state equation (63) is given by

$$\text{if } \gamma_1^2-\gamma_3^2+x_{A3}^2<0 \qquad \mathcal{D}^{(\rightarrow)}(\rho_{AB})=\frac{|\gamma_1|}{2},$$

$$\text{if } \gamma_1^2-\gamma_3^2+x_{A3}^2\geqslant 0 \begin{cases} \text{if } |\gamma_3|\geqslant|\gamma_1|, \quad \mathcal{D}^{(\rightarrow)}(\rho_{AB})=\frac{|\gamma_1|}{2} \\ \text{if } |\gamma_3|<|\gamma_1|, \quad \mathcal{D}^{(\rightarrow)}(\rho_{AB})=\Theta\left(\gamma_2^2-\gamma_3^2+x_{A3}^2\right)\frac{1}{2}\sqrt{\frac{\gamma_1^2(\gamma_2^2+x_{A3}^2)-\gamma_2^2\gamma_3^2}{\gamma_1^2-\gamma_3^2+x_{A3}^2}} \\ \qquad\qquad +\Theta\left[-\left(\gamma_2^2-\gamma_3^2+x_{A3}^2\right)\right]\frac{|\gamma_3|}{2}, \end{cases} \tag{65}$$

where we have used the Heaviside step function $\Theta(x)$ (we adopt the standard convention $\Theta(0)=1/2$). It can be checked (see appendix B) that for Bell-diagonal states the above expression reproduces the result of section 3; that is, the TDD is half the intermediate value among $\{|\gamma_k|\}$ (we stress that here the labeling of the γ_k's does not imply the ordering in equation (33)).

Equation (65) can also be written in the compact form

$$\mathcal{D}^{(\rightarrow)}(\rho_{AB})=\frac{1}{2}\sqrt{\frac{\gamma_1^2\ \max\{\gamma_3^2,\gamma_2^2+x_{A3}^2\}-\gamma_2^2\ \min\{\gamma_3^2,\gamma_1^2\}}{\max\{\gamma_3^2,\gamma_2^2+x_{A3}^2\}-\min\{\gamma_3^2,\gamma_1^2\}+\gamma_1^2-\gamma_2^2}} \tag{66}$$

showing that, for the X-states, the discord is only a function of the following three parameters: $|\gamma_1|$, $|\gamma_3|$ and $\sqrt{\gamma_2^2+x_{A3}^2}$.

To begin with, equations (28) and (29) imply that the (θ,ϕ)-dependent functions a and b entering equation (31) (recall that (θ,ϕ) specify $\hat{e}$) depend only on $\mu\equiv\sin^2\theta$ and $\nu\equiv\sin^2\phi$ as

$$a=a_0+a_1\,\mu, \qquad b=b_0+b_1\,\mu+b_2\,\mu^2, \tag{67}$$

where $\{a_i\}$ and $\{b_i\}$ are the following linear functions of ν:

$$a_0=\gamma_1^2+\gamma_2^2, \qquad a_1=(\gamma_3^2+x_{A3}^2-\gamma_1^2)+(\gamma_1^2-\gamma_2^2)\nu, \tag{68}$$

$$b_0=4\gamma_1^2\gamma_2^2, \qquad b_2=4x_{A3}^2\left[(\gamma_3^2-\gamma_1^2)+(\gamma_1^2-\gamma_2^2)\nu\right], \tag{69}$$

$$b_1=4\left[\gamma_2^2\gamma_3^2+\gamma_1^2(x_{A3}^2-\gamma_2^2)+(\gamma_1^2-\gamma_2^2)(\gamma_3^2-x_{A3}^2)\nu\right]. \tag{70}$$

Clearly, $a(\mu,\nu)$ and $b(\mu,\nu)$ are defined in the square $\mathcal{S}\equiv\{\mu,\nu:0\leqslant\mu\leqslant 1,0\leqslant\nu\leqslant 1\}$ (and so is $h=a+\sqrt{a^2-b}$, see equation (31)). The partial derivative of h with respect to ν, $\partial_\nu h$, can be arranged as $\partial_\nu h=(2\,h\partial_\nu a-\partial_\nu b)/(2\sqrt{a^2-b})$ (an analogous formula holds for $\partial_\mu h$). Now, due to equations (67)–(70) $\partial_\nu a=(\gamma_1^2-\gamma_2^2)\mu$ and, notably, $\partial_\nu b=4[\gamma_3^2+(\mu-1)x_{A3}^2]\partial_\nu a$. When these are replaced in $\partial_\nu h$ we, thus, end up with

$$\partial_\nu h=\frac{h-2\left[\gamma_3^2+x_{A3}^2(\mu-1)\right]}{\sqrt{a^2-b}}\ \partial_\nu a. \tag{71}$$

As witnessed by the denominator of this equation, we observe that function h is in general non-differentiable at points such that $a^2=b$, owing to the square root $\sqrt{a^2-b}$ appearing in its definition, equation (31). One then has to investigate these points carefully because they may yield extremal values of h that would not be found by simply imposing $\partial_\mu h=\partial_\nu h=0$.

As a key step in our reasoning, we first demonstrate that *a minimum of h cannot occur in the interior of $\mathcal{S}$*. Afterwards, we minimize function h on the boundary of $\mathcal{S}$, which will eventually lead to formula (65).

5.1. Proof that minimum points cannot lie in the interior of $\mathcal{S}$

We first address minimum points at which h is differentiable; that is, that fulfil $a^2 \neq b$ entailing the existence of partial derivatives for h. A necessary condition for h to take a minimum on these points is then $\partial_\nu h = 0$. Based on equation (71), this can happen when either $h = h_0 = 2[\gamma_3^2 + x_{A3}^2(\mu - 1)]$ or $\partial_\nu a = 0$.

In the latter case, as discussed above, $\partial_\nu a = (\gamma_1^2 - \gamma_2^2)\mu$, which vanishes for $\mu = 0$ (that is, on the boundary of $\mathcal{S}$) or $|\gamma_1| = |\gamma_2|$. Using equations (31) and (67) through (70) it is easy to calculate that when $|\gamma_1| = |\gamma_2|$, depending on the sign of $\gamma_2^2 - \gamma_3^2 + x_{A3}^2$, either $h = 2(\gamma_2^2 + x_{A3}^2\mu)$ or $2[\gamma_2^2 + (\gamma_3^2 - \gamma_2^2)\mu]$. Thereby, in the case $|\gamma_1| = |\gamma_2|$ the minima of h must fall on the boundary of $\mathcal{S}$.

Let us now analyze the situation where $h = h_0 = 2[\gamma_3^2 + x_{A3}^2(\mu - 1)]$, which would also yield $\partial_\nu h = 0$ (cf equation (71)). Since $h = a + \sqrt{a^2 - b}$, a necessary condition for this to occur is clearly $(h_0 - a)^2 = a^2 - b$. With the help of equations (67)–(70), this identity can be explicitly written as $4(1-\mu)(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)(\gamma_2^2 - \gamma_3^2 + x_{A3}^2) = 0$. This is fulfilled if at least one of the following identities holds: (i) $\mu = 1$; (ii) $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 = 0$; and (iii) $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 = 0$. Case (i) clearly corresponds to a point on the boundary of $\mathcal{S}$. In case (ii), using that $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \leqslant 0$ (due to $\gamma_2^2 \leqslant \gamma_1^2 = \gamma_3^2 - x_{A3}^2$) we end up with $h = 2[(\gamma_3^2 - x_{A3}^2) + x_{A3}^2\mu]$. In case (iii), using that $\gamma_!1^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0$ (due to $\gamma_1^2 \geqslant \gamma_2^2 = \gamma_3^2 - x_{A3}^2$) we have that $h = 2\{\gamma_1^2 + [\gamma_3^2 - \gamma_1^2 + (\gamma_1^2 - \gamma_3^2 + x_{A3}^2)\nu]\mu\}$, whose minimum occurs for $\mu = \nu = 0$ or $\mu = 1$ and $\nu = 0$ (depending on the sign of $\gamma_3^2 - \gamma_1^2$). Hence, even in cases (ii) and (iii), the minima of h fall on the boundary of $\mathcal{S}$. This shows that no minima points at which h is differentiable can lie in the interior $\mathcal{S}$.

Let us now address singular points; that is, those at which h is non-differentiable and, hence, minimization criteria based on partial derivatives do not apply. These points (see above discussion) are the zeros of the function $f = a^2 - b$. Our aim is to prove that even such points, if they exist, lie on the boundary of $\mathcal{S}$. Firstly, note that $f \geqslant 0$ (we recall that $a^2 \geqslant b$ always holds, see section 2). This means that a zero of f is also a minimum point for f. From equations (67)–(70), it is evident that $f(\mu, \nu)$ is analytic throughout the real plane. Then, a necessary condition for this function to take a minimum is $\partial_\mu f = \partial_\nu f = 0$. It is easy to check that $\partial_\nu f$ is a simple second-degree polynomial in μ, with zeros $\mu_{s1} = 0$ and $\mu_{s2} = (\gamma_1^2 + \gamma_2^2 - 2\gamma_3^2 + 2x_{A3}^2)/[(\gamma_1^2 - \gamma_3^2 + x_{A3}^2) + (\gamma_2^2 - \gamma_1^2)\nu]$. The former solution clearly cannot correspond to stationary points of f—in particular zeros of f, that is, *singular points of* h—that lie in the interior of $\mathcal{S}$ (as anticipated, a zero of f is also a minimum and, thus, one of its stationary points). On the other hand, by plugging μ_{s2} into $\partial_\mu f$ we find $\partial_\mu f|_{\mu=\mu_{s2}} = 4(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)(\gamma_2^2 - \gamma_3^2 + x_{A3}^2)$, which vanishes for either $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 = 0$ or $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 = 0$. We have already shown (see above) that in neither of these two cases can h admit minima in the interior of $\mathcal{S}$.

5.2. Minima on the boundary of $\mathcal{S}$

The findings of the previous subsection show that we can restrict the search for the minimum of h to the boundary of $\mathcal{S}$. The possible values of h on the square edges corresponding to $\mu = 0$, $\mu = 1$, $\nu = 0$ and $\nu = 1$ are, respectively, given by

$$h_{\mu=0} = \gamma_1^2 + \gamma_2^2 + \left|\gamma_1^2 - \gamma_2^2\right| = 2\gamma_1^2, \tag{72}$$

$$h_{\mu=1} = \gamma_3^2 + x_{A3}^2 + \gamma_2^2 + (\gamma_1^2 - \gamma_2^2)\nu + \left|\gamma_2^2 - \gamma_3^2 + x_{A3}^2 + (\gamma_1^2 - \gamma_2^2)\nu\right|, \tag{73}$$

$$h_{\nu=0} = \gamma_2^2 + \gamma_1^2 - (\gamma_1^2 - \gamma_3^2 - x_{A3}^2)\mu + \left|\gamma_2^2 - \gamma_1^2(1-\mu) + (x_{A3}^2 - \gamma_3^2)\mu\right|, \tag{74}$$

$$h_{\nu=1} = \gamma_2^2 + \gamma_1^2 - (\gamma_2^2 - \gamma_3^2 - x_{A3}^2)\mu + \left|\gamma_1^2 - \gamma_2^2(1-\mu) + (x_{A3}^2 - \gamma_3^2)\mu\right|. \tag{75}$$

From equation (72), it trivially follows that the minimum of h on edge $\mu = 0$ is given by $\min h_{\mu=0} = 2\gamma_1^2$. In the next three dedicated paragraphs, we minimize h on edges $\mu = 1$ and $\nu = 0, 1$.

5.2.1. Edge $\mu = 1$. This is the set of points ($\mu = 1, 0 \leqslant \nu \leqslant 1$) on which function h is given by equation (73). Let h_+ (h_-) be the expression taken by h when the absolute value in equation (73) is positive (negative). These are easily calculated as

$$h_+(\nu) = 2\left[\gamma_2^2 + x_{A3}^2 + (\gamma_1^2 - \gamma_2^2)\nu\right], \quad h_-(\nu) = 2\gamma_3^2. \tag{76}$$

Importantly, note that h_+ always grows with ν while h_- is flat.

The argument of the absolute value (cf equation (73)) increases with ν (since $\gamma_1^2 \geqslant \gamma_2^2$) and vanishes for $\nu = \nu_0 = -(\gamma_2^2 - \gamma_3^2 + x_{A3}^2)/(\gamma_1^2 - \gamma_2^2)$. Hence, it is negative (non-negative) for $\nu < \nu_0$ ($\nu \geqslant \nu_0$). Consequently, $h = h_-$ ($h = h_+$) for $\nu < \nu_0$ ($\nu \geqslant \nu_0$). Now, the minimum of h on this edge depends on the sign of ν_0, which depends in turn on the sign of $\gamma_2^2 - \gamma_3^2 + x_{A3}^2$. Indeed, if $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0$ then $\nu_0 > 0$ and thus $\min h_{\mu=1} \equiv \min h_- = 2\gamma_3^2$ (recall that h_+ grows with ν). If, instead, $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0$ then $\nu_0 \leqslant 0$ and $h \equiv h_+$ for $0 \leqslant \nu \leqslant 1$, namely throughout the edge. The minimum is thus taken at $\nu = 0$ and reads $\min h_{\mu=1} \equiv \min h_+(\nu = 0) = 2(\gamma_2^2 + x_{A3}^2)$. To summarize,

$$\text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0 \quad \min h_{\mu=1} = 2\gamma_3^2, \tag{77}$$

$$\text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0 \quad \min h_{\mu=1} = 2(\gamma_2^2 + x_{A3}^2), \tag{78}$$

5.2.2. Edge $\nu = 0$. This is the set of points ($0 \leqslant \mu \leqslant 1$, $\nu = 0$), where h is given by equation (74). Similarly to the previous paragraph, we first search for the zero of the absolute value, which is easily found as $\mu = \mu_0 = (\gamma_1^2 - \gamma_2^2)/(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)$. Its location on the real axis fulfils

$$\text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0 \begin{cases} \text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0, & 0 \leqslant \mu_0 \leqslant 1, \\ \text{if } \gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0, & \mu_0 > 1, \end{cases} \tag{79}$$

$$\text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0, \quad \mu_0 < 0, \tag{80}$$

which we will use in our analysis. At variance with the previous paragraph, now the absolute value in equation (74) grows (decreases) with μ for $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0$ ($\gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0$). Equation (73) straightforwardly gives

$$h_+(\mu) = 2(\gamma_2^2 + x_{A3}^2\,\mu), \quad h_-(\mu) = 2\left[\gamma_1^2 + (\gamma_3^2 - \gamma_1^2)\,\mu\right], \tag{81}$$

where $h_\pm$ are defined in full analogy with the previous paragraph. Note that, while h_+ always grows with μ, h_- is an increasing (decreasing) function of μ for $|\gamma_3| \geqslant |\gamma_1|$ ($|\gamma_3| < |\gamma_1|$). Let us analyze the possible situations. Based on the above, if $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0$ then $\mu_0 \geqslant 0$ and, moreover, the absolute value is negative (non-negative) for $\mu < \mu_0$ ($\mu \geqslant \mu_0$). This yields $h(\mu < \mu_0) = h_-$ and $h(\mu \geqslant \mu_0) = h_+$. Now, two cases can occur. If $|\gamma_3| \geqslant |\gamma_1|$, then h_- grows with μ and, therefore, $\min h_{\nu=0} \equiv h_-(\mu = 0) = 2\gamma_1^2$. If $|\gamma_3| < |\gamma_1|$, instead, h_- decreases with

μ. Then, the minimum of h depends on whether or not $\mu_0 \leqslant 1$, which depends in turn on the sign of $\gamma_2^2 - \gamma_3^2 + x_{A3}^2$ according to equation (79). If $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0$ then $\mu_0 \leqslant 1$ and h is minimized for $\mu = \mu_0$ (recall that h_+ always grows). This yields $\min h_{\nu=0} \equiv h_-(\mu_0) = 2\,[\gamma_1^2(\gamma_2^2 + x_{A3}^2) - \gamma_2^2\gamma_3^2]/(\gamma_1^2 - \gamma_3^2 + x_{A3}^2)$. On the other hand, $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0$ implies $\mu_0 > 1$. Hence, $h \equiv h_-$ throughout the interval $0 \leqslant \mu \leqslant 1$ and, necessarily, $\min h_{\nu=0} \equiv h_-(\mu = 1) = 2\gamma_3^2$.

We are left with the case $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0$. In this situation, $\mu_0 < 0$ (cf equation (80)) and the absolute value is non-negative (negative) for $\mu \leqslant \mu_0$ ($\mu > \mu_0$), which gives $h \equiv h_-$ throughout this edge. Now, the analysis is simpler since, evidently, only the case $|\gamma_1| < |\gamma_3|$ is possible. Thus, h_- can only increase (recall equation (81)) and $\min h_{\nu=0} = h_-(\mu = 0) = 2\gamma_1^2$.

To summarize, on the edge $\nu = 0$

$$\text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 < 0 \qquad \min h_{\nu=0} = 2\gamma_1^2 \ , \tag{82}$$

$$\text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0 \begin{cases} \text{if } |\gamma_3| \geqslant |\gamma_1| & \min h_{\nu=0} = 2\gamma_1^2, \\ \text{if } |\gamma_3| < |\gamma_1| & \min h_{\nu=0} = \Theta\left(\gamma_2^2 - \gamma_3^2 + x_{A3}^2\right) 2\frac{\gamma_1^2(\gamma_2^2 + x_{A3}^2) - \gamma_2^2\gamma_3^2}{\gamma_1^2 - \gamma_3^2 + x_{A3}^2} \\ & \quad + \Theta\left[-\left(\gamma_2^2 - \gamma_3^2 + x_{A3}^2\right)\right] 2\gamma_3^2. \end{cases} \tag{83}$$

5.2.3. Edge $\nu = 1$. This is the set of points ($0 \leqslant \mu \leqslant 1$, $\nu = 1$), where h is given by equation (75). Similarly to the previous paragraph, we first search for the zero of the absolute value, which is easily found as $\mu = \mu_0 = -(\gamma_1^2 - \gamma_2^2)/(\gamma_2^2 - \gamma_3^2 + x_{A3}^2)$. Its location on the real axis fulfils

$$\text{if } \ \gamma_2^2 - \gamma_3^2 + x_{A3}^2 > 0, \qquad \mu_0 < 0 \ , \tag{84}$$

$$\text{if } \ \gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0 \begin{cases} \text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 > 0, & \mu_0 > 1, \\ \text{if } \gamma_1^2 - \gamma_3^2 + x_{A3}^2 \leqslant 0, & 0 \leqslant \mu_0 \leqslant 1. \end{cases} \tag{85}$$

Based on equation (75), the expressions taken by h on this edge when the absolute value is positive and negative are, respectively

$$h_+(\mu) = 2(\gamma_1^2 + x_{A3}^2\,\mu), \quad h_-(\mu) = 2\left[\gamma_2^2 + (\gamma_3^2 - \gamma_2^2)\,\mu\right]. \tag{86}$$

Hence, h_+ always grows with μ while h_- is an increasing (decreasing) function of μ for $|\gamma_3| \geqslant |\gamma_2|$ ($|\gamma_3| < |\gamma_2|$). We show next that the minimum of h on this edge is always given by $2\gamma_1^2$.

Indeed, if $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0$ (implying $\gamma_1^2 - \gamma_3^2 + x_{A3}^2 \geqslant 0$) then $\mu_0 \leqslant 0$ and $h \equiv h_+(\mu)$ throughout the edge. The minimum is, thus, $\min h_{\nu=1} = h_+(0) = 2\gamma_1^2$. If, instead, $\gamma_2^2 - \gamma_3^2 + x_{A3}^2 < 0$ then $h = h_+$ ($h = h_-$) for $\mu \leqslant \mu_0$ ($\mu > \mu_0$). Moreover, note that in this case one has $\gamma_3^2 > \gamma_2^2$, which entails (cf equation (86)) that both h_- and h_+ grow with μ. Hence, the minimum is again given by $\min h_{\nu=1} = h_+(0) = 2\gamma_1^2$, which completes our proof.

5.3. Global minimum

To give the general expression for the minimum of h, it is convenient to refer to the minimization study on the edge $\nu = 0$. Recall that the minimum of h on the edges $\mu = 0$ and $\nu = 1$ is

unconditionally given by $2\gamma_1^2$. When $\gamma_1^2-\gamma_3^2+x_{A3}^2<0$, based on equations (77) and (82) the minimum reads $\min_{\hat{e}} h=2\gamma_1^2$ (note indeed that this case necessarily entails $\gamma_2^2-\gamma_3^2+x_{A3}^2<0$ and $\gamma_1^2<\gamma_3^2$). If instead $\gamma_1^2-\gamma_3^2+x_{A3}^2\geqslant 0$, then both signs of $\gamma_2^2-\gamma_3^2+x_{A3}^2$ as well as $|\gamma_3|-|\gamma_1|$ are possible. Hence, if $|\gamma_3|\geqslant|\gamma_1|$ upon analysis of equations (77) and (78) and the first case in equation (83) we end up with $\min_{\hat{e}} h=\min\{2\gamma_1^2, 2(\gamma_2^2+x_{A3}^2)\}$. Let us now consider $|\gamma_3|<|\gamma_1|$. For $\gamma_2^2-\gamma_3^2+x_{A3}^2<0$, this gives $\min_{\hat{e}} h=2\gamma_3^2$. For $\gamma_2^2-\gamma_3^2+x_{A3}^2\geqslant 0$, the global minimum is the lowest number among $2\gamma_1^2$, $2(\gamma_2^2+x_{A3}^2)$ and $2[\gamma_1^2(\gamma_2^2+x_{A3}^2)-\gamma_2^2\gamma_3^2]/(\gamma_1^2-\gamma_3^2+x_{A3}^2)$. Hence, to summarize,

$$
\begin{aligned}
&\text{if } \gamma_1^2-\gamma_3^2+x_{A3}^2<0 \qquad\qquad \min h=2\gamma_1^2,\\
&\text{if } \gamma_1^2-\gamma_3^2+x_{A3}^2\geqslant 0\\
&\begin{cases}
\text{if } |\gamma_3|\geqslant|\gamma_1| & \min h=\Theta(\gamma_2^2-\gamma_3^2+x_{A3}^2)\,2\min\left\{\gamma_1^2,\gamma_2^2+x_{A3}^2\right\}\\
& \qquad +\Theta\left[-(\gamma_2^2-\gamma_3^2+x_{A3}^2)\right]2\gamma_1^2,\\
\text{if } |\gamma_3|<|\gamma_1| & \min h=\Theta(\gamma_2^2-\gamma_3^2+x_{A3}^2)2\min\left\{\gamma_1^2,\gamma_2^2+x_{A3}^2,\frac{\gamma_1^2(\gamma_2^2+x_{A3}^2)-\gamma_2^2\gamma_3^2}{\gamma_1^2-\gamma_3^2+x_{A3}^2}\right\}\\
& \qquad +\Theta\left[-\left(\gamma_2^2-\gamma_3^2+x_{A3}^2\right)\right]2\gamma_3^2.
\end{cases}
\end{aligned}
\tag{87}
$$

Equation (87) can be further simplified. Indeed, on the second line (case $\gamma_1^2-\gamma_3^2+x_{A3}^2\geqslant 0$ and $|\gamma_3|\geqslant|\gamma_1|$) for $\gamma_2^2-\gamma_3^2+x_{A3}^2\geqslant 0$ we have $\gamma_2^2+x_{A3}^2\geqslant\gamma_3^2\geqslant\gamma_1^2$ and, therefore, the minimum is $2\gamma_1^2$ regardless of $\gamma_2^2+x_{A3}^2\geqslant\gamma_3^2$. On the other hand, on the third line (case $\gamma_1^2-\gamma_3^2+x_{A3}^2\geqslant 0$ and $|\gamma_3|<|\gamma_1|$) for $\gamma_2^2-\gamma_3^2+x_{A3}^2\geqslant 0$ and using $\gamma_1^2\geqslant\gamma_2^2$ it is straightforward to prove that the rational function can never exceed both γ_1^2 and $\gamma_2^2+x_{A3}^2$. In light of these considerations, and upon comparison of equation (87) with equations (82) and (83), we conclude that the global minimum of h is achieved on the edge $\nu=0$. Therefore, using equation (32) the TDD of an arbitrary two-qubit X state is finally obtained as in equation (65). Remarkably, in each case that can occur (depending on the parameters defining the state) $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ takes a relatively compact expression.

As already anticipated, for Bell-diagonal states (see section 3), equation (65) yields the result of section 3.1, as shown in detail in appendix B.

Another interesting special case occurs when in equation (63) either $\rho_{32}=0$ or $\rho_{41}=0$. Then, due to equation (64), $|\gamma_1|\equiv|\gamma_2|$ and $\sqrt{\frac{\gamma_1^2(\gamma_2^2+x_{A3}^2)-\gamma_2^2\gamma_3^2}{\gamma_1^2-\gamma_3^2+x_{A3}^2}}\rightarrow\frac{|\gamma_2|}{2}$. Hence, such a case always entails $\mathcal{D}^{(\rightarrow)}(\rho_{AB})=|\gamma_1|/2$, namely half of the absolute value of the non-zero off-diagonal entry.

6. Application: propagation of quantum correlations across a spin chain

In this section, we present an illustrative application of our findings to a concrete problem of QCs dynamics. The problem was investigated in [33] and regards the propagation dynamics of QCs along a spin chain. Specifically, consider a chain of N qubits, each labeled by index $i=1,\cdots,N$ with an associated Hamiltonian

$$
H=-2\,J\sum_{i=1}^{N-1}\left(\sigma_{i1}\sigma_{i+1,1}+\sigma_{i2}\sigma_{i+1,2}\right). \tag{88}
$$

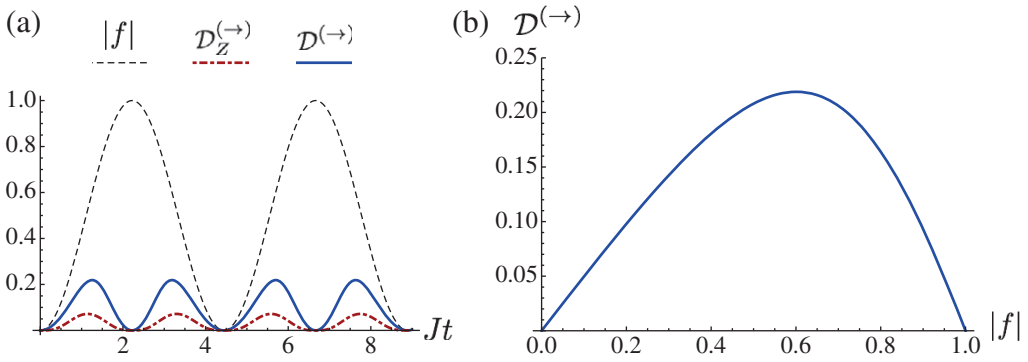

Figure 2. (a) Absolute value of the transfer amplitude $|f|$ (black dashed line), quantum discord $\mathcal{D}_Z^{(\rightarrow)}$ (red dot-dashed) and TDD $D^{(\rightarrow)}$ (blue solid) against time (in units of J^{-1}) for $N = 3$. (b) Functional relationship between TDD and $|f|$ as given by equation (91).

Such an XX model is routinely used to investigate quantum state transfer [34]. An additional qubit, disconnected from the chain and denoted by $i = 0$, initially shares QCs with the first qubit of the chain corresponding to $i = 1$ (with each of the remaining qubits initially prepared in state $|0\rangle$). The problem consists in studying how the bipartite QCs between qubits 0 and r with $r = 1, \ldots, N$ evolve in time. If $r = N$, in particular, one can regard this process as the end-to-end propagation of QCs across the spin chain. In [33], the authors found a number of interesting properties, especially in comparison with the corresponding entanglement propagation. To carry out their analysis, they used the quantum discord $\mathcal{D}_Z^{(\rightarrow)}$ [2]. For the specific two-qubit states involved in such dynamics, $\mathcal{D}_Z^{(\rightarrow)}$ can be calculated analytically. Yet, this circumstance does not yield any advantage in practice since the resulting formulae are lengthy and uninformative, as pointed out by the authors themselves [33]. We next provide evidence that, if instead of $\mathcal{D}_Z^{(\rightarrow)}$, one uses the TDD $\mathcal{D}^{(\rightarrow)}$ then simple and informative formulas arise.

It is easily demonstrated [33] that if $\rho_{10} = (\mathbb{I}_{10} + \sigma_{11}\sigma_{01})/4$ is the initial state of qubits 1 and 0, then at time t the state of N and 0 reads

$$\rho_{N0}(t) = \begin{pmatrix} \frac{2-|f(t)|^2}{4} & 0 & 0 & \frac{f(t)}{4} \\ 0 & \frac{2-|f(t)|^2}{4} & \frac{f(t)}{4} & 0 \\ 0 & \frac{f^*(t)}{4} & \frac{|f(t)|^2}{4} & 0 \\ \frac{f^*(t)}{4} & 0 & 0 & \frac{|f(t)|^2}{4} \end{pmatrix}, \tag{89}$$

where $f(t)$ is the single-excitation transition amplitude given by

$$f(t) = \frac{2}{N+1} \sum_{k=1}^{N} \sin \frac{k\pi}{N+1} \sin \frac{k\pi N}{N+1} e^{-2iJ \cos \frac{k\pi}{N+1} t}. \tag{90}$$

Therefore, f fully specifies the output state (89) and, thus, any corresponding QCs measure. Figure 2(a) shows, in particular, the behavior of $|f(t)|$ and $\mathcal{D}_Z^{(\rightarrow)}[f((t)]$ for $N = 3$, which fully reproduces the results in [33] (in absence of a magnetic field). The quantum discord is evidently a non-monotonic function of $|f|$, which vanishes for $|f| = 0, 1$ exhibiting a single maximum at

an intermediate value of $|f|$. There appears to be no straightforward way to prove this behavior since, as anticipated, function $\mathcal{D}_Z^{(\rightarrow)}(f)$ has a complicated analytical form.

Let us now calculate $\mathcal{D}^{(\rightarrow)}(f)$. The state in equation (89) is an X state, hence, our techniques of section 5 can be applied to calculate the corresponding TDD[11]. Using the notation of section 5, and observing that off-diagonal entries in equation (89) can be replaced by their moduli (up to local unitaries that do not affect TDD), we find $\gamma_1 = |f(t)|$, $\gamma_2 = \gamma_3 = 0$ and $x_{A3} = 1 - |f(t)|^2$. Substituting these in equation (66) then yields the compact expression

$$\mathcal{D}^{(\rightarrow)}(f) = \frac{1}{2}\frac{|f|\,(1-|f|^2)}{\sqrt{|f|^4 - |f|^2 + 1}}, \tag{91}$$

which is plotted in figure 2(b). Once f is expressed as a function of time with the help of equation (90) we obtain the non-monotonic time behavior of $\mathcal{D}^{(\rightarrow)}$ displayed in figure 2(a). This exhibits the same qualitative features as $\mathcal{D}_Z^{(\rightarrow)}(t)$, which shows that TDD has a predictive power analogous to the quantum discord. Unlike the latter, though, acquiring analytical insight is now straightforward. Indeed, it is immediate to see from equation (91) that $\mathcal{D}^{(\rightarrow)}$ vanishes for $|f| = 0, 1$. Moreover, the equation $\mathrm{d}\mathcal{D}^{(\rightarrow)}/\mathrm{d}|f| = 0$ (which is easily seen to be equivalent to an effective third-degree equation) admits only one root in the range $[0, 1]$ given by $|f|_{\mathrm{M}} \simeq 1/\sqrt{3/(1 - 8/\tau + \tau)} \simeq 0.6$ with $\tau = (1 + 3\sqrt{57})^{1/3}$. As $\mathrm{d}\mathcal{D}^{(\rightarrow)}/\mathrm{d}|f| > 0$ for $|f| = 0$, the TDD takes a maximum at $|f| = |f|_{\mathrm{M}}$ given by $\mathcal{D}_{\mathrm{M}}^{(\rightarrow)} = \mathcal{D}^{(\rightarrow)}(|f|_{\mathrm{M}}) \simeq 0.22$ (see figure 2(b)).

This paradigmatic instance illustrates the effectiveness of our findings as a tool to acquire readable and reliable informations on QCs in a concrete physical problem.

7. Conclusions

In this paper, we have addressed the issue of the computability of TDD, which is one of the most reliable and advantageous QCs indicators. By introducing a new method for tackling and simplifying the minimization required for its calculation in the two-qubit case, we have demonstrated that this can be reduced to the search for the minimum of an explicit two-variable function. Then, we have shown that this can be analytically found in a closed form for some relevant classes of states, which encompass arbitrary quantum-classical and X states. The latter includes the Bell diagonal states as a special subset, which were the only states for which an analytical expression of TDD had been worked out prior to our work. Our results are summarized in table 1. Finally, we have illustrated the effectiveness of our findings in a specific paradigmatic problem where, despite being achievable, the analytical calculation of quantum discord is not informative. In contrast, TDD is readily calculated in a simple explicit form, being able at the same time to capture all the salient physical features of the QCs dynamics. Such an approach could, therefore, prove particularly useful in order to clarify the role and physical meaning of QCs in a number of quantum coherent phenomena.

Due to the importance of quantum-classical and X states, along with the typical hindrances to the calculation of their QCs through bona fide measures, our work provides a significant contribution to the study of QCs quantifiers by combining the desirable mathematical properties of TDD with its explicit computation for these classes of density matrices. Furthermore, we expect that the framework developed in this paper may be further exploited in future

[11] It can be shown that in line with [33] state (89) is quantum-classical too, hence the formulae in section 4.1 can also be used. It is however more immediate to use those in section 5.

Table 1. Summary of the main results of the paper. We recall that the γ_j's indicate the (real) singular values of the correlation matrix Γ, with associated unit vectors $\hat{w}_j$, while $\vec{x}_A$ is the local Bloch vector of subsystem A, expressed in the coordinate system $\{\hat{w}_j\}_{j=1}^3$—see section 2.

Summary of results	
Section 3	
Bell diagonal states and states with uniform singular values[a]	$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{\lvert\gamma_2\rvert}{2}$
Example: $\rho_{AB} = p\varrho_A \mathbf{1}_B/2 + (1-p)\lvert\Psi_-\rangle\langle\Psi_-\rvert$	$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{1-p}{2}$
Section 4	
Rank-one correlation matrix ($\vec{\gamma}_1 \equiv \gamma_1 \hat{w}_1$)	$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{\lvert\vec{\gamma}_1 \wedge \vec{x}_A\rvert}{2} \min\left\{\frac{1}{\lvert\vec{\gamma}_1 \pm \vec{x}_A\rvert}\right\}$,
Example: QC states (section 4.1)[b]	$\mathcal{D}^{(\rightarrow)}(\rho_{AB}) = \frac{\sin\varphi}{2} \min\{ps_0, (1-p)s_1\}$,
Section 5	
X states[c]	$\mathcal{D}^{(\rightarrow)}(\rho_{\mathrm{AB}}) = \frac{1}{2}\sqrt{\frac{\gamma_1^2 \max\{\gamma_3^2, \gamma_2^2 + x_{A3}^2\} - \gamma_2^2 \min\{\gamma_3^2, \gamma_1^2\}}{\max\{\gamma_3^2, \gamma_2^2 + x_{A3}^2\} - \min\{\gamma_3^2, \gamma_1^2\} + \gamma_1^2 - \gamma_2^2}}$

[a] In section 3, the ordering $|\gamma_1| \geqslant |\gamma_2| \geqslant |\gamma_3|$ is assumed.
[b] We recall the standard form of a quantum-classical state: $\rho_{AB} = p\,\rho_{0A} \otimes |0\rangle_B\langle 0| + (1-p)\rho_{1A} \otimes |1\rangle_B\langle 1|$, where $\vec{s}_j$ is the Bloch vector of ρ_{jA}, $s_j = |\vec{s}_j|$ $(j = 0, 1)$ and φ is the smallest angle between $\vec{s}_0$ and $\vec{s}_1$.
[c] In section 5, $|\gamma_1| \geqslant |\gamma_2|$ is assumed, while no assumption is made on $|\gamma_3|$.

investigations to enlarge the class of quantum states that admit an analytical expression for TDD.

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Appendix A. Derivation of equation (48)

We recall that $f_\pm(\phi, \alpha) = \gamma \cos\phi \pm x_A \cos(\phi - \alpha)$. This is a linear combination of $\cos\phi$ and $\sin\phi$, which can be arranged in terms of a single cosine as $A_\pm(\cos\phi\cos\delta_\pm + \sin\phi\sin\delta_\pm) = A_\pm\cos(\phi - \delta_\pm)$. Using $\tilde{x}_{A1} = x_A\cos\alpha$ (see equation (44)), the factor is easily found as $A_\pm = \sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}$, while

$$\sin\delta_\pm = \frac{\pm x_A \sin\alpha}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}} = \frac{\pm\tilde{x}_{A2}}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}}, \tag{A.1}$$

$$\cos\delta_\pm = \frac{\gamma \pm x_A\cos\alpha}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}} = \frac{\gamma \pm \tilde{x}_{A1}}{\sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}}. \tag{A.2}$$

Hence, $\delta_\pm = \arctan\left[\tilde{x}_{A2}/(\tilde{x}_{A1} \pm \gamma)\right]$. Therefore

$$f_\pm(\phi, \alpha) = \sqrt{(\gamma \pm \tilde{x}_{A1})^2 + \tilde{x}_{A2}^2}\ \cos(\phi - \delta_\pm). \tag{A.3}$$

Replacing equation (A.3) into equation (47) of the main text yields

$$\begin{aligned}\|M(\hat{e})\|_1 &= 2\sum_{\eta=\pm}\sqrt{\left[(\gamma+\eta\tilde{x}_{A1})^2+\tilde{x}_{A2}^2\right]\left[1-\cos^2(\phi-\delta_\eta)\right]}\\ &= 2\sum_{\eta=\pm}\sqrt{(\gamma+\eta\tilde{x}_{A1})^2+\tilde{x}_{A2}^2}\;|\sin(\phi-\delta_\eta)|\\ &= 2\sum_{\eta=\pm}\sqrt{(\gamma+\eta\tilde{x}_{A1})^2+\tilde{x}_{A2}^2}\;|\sin\phi\cos\delta_\eta-\cos\phi\sin\delta_\eta|.\end{aligned}$$

Eliminating now $\sin\delta_\pm$ and $\cos\delta_\pm$ through equations (A.1) and (A.2) we end up with equation (48) of the main text.

Appendix B. Equation (65) for Bell diagonal states

Bell diagonal states are defined as a mixture of the four Bell states. This immediately yields that they fulfil $\vec{x}_A=\vec{x}_B=0$, that is, the reduced density matrix describing the state of either party is maximally mixed. Therefore, the corresponding density matrix can be expanded as a linear combination of $\mathbb{I}_A\otimes\mathbb{I}_B$ and $\{\sigma_{Ak}\otimes\sigma_{Bk}\}$. As each of these four operators has an X-form matrix representation (cf equation (63)) Bell-diagonal states are X states. Hence, in equation (65) $\gamma_i^2-\gamma_3^2+x_{A3}^2\to\gamma_i^2-\gamma_3^2$ for $i=1,2$. In this case, the square root in equation (65) coincides with $|\gamma_2|$ and the TDD reduces to

$$\begin{aligned}&|\gamma_3|\geqslant|\gamma_1|\Rightarrow\mathcal{D}^{(\rightarrow)}(\rho_{AB})=\frac{|\gamma_1|}{2},\\ &|\gamma_3|<|\gamma_1|\Rightarrow\mathcal{D}^{(\rightarrow)}(\rho_{AB})=\tfrac{1}{2}\max\{|\gamma_2|,|\gamma_3|\}.\end{aligned}\tag{B.1}$$

It is immediate to check that the above is equivalent to state that $\mathcal{D}^{(\rightarrow)}(\rho_{AB})$ is half of the *intermediate* value among $\{|\gamma_1|,|\gamma_2|,|\gamma_3|\}$, which fully agrees with [16, 17] and the findings of section 3.1.

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