Geometric quantum discord of an arbitrary two-qudit state: Exact value and general upper bounds

Elena R. Loubenets * and Louis Hanotel
Department of Applied Mathematics, HSE University, Moscow 101000, Russia

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The geometric quantum discord of a two-qudit state has been studied in many papers; however, its exact analytical value in the explicit form is known only for a general two-qubit state, a general qubit-qudit state, and some special families of two-qudit states. Based on the general Bloch vectors formalism [E. R. Loubenets *et al.*, J. Phys. A: Math. Theor. **54**, 195301 (2021)], we find the explicit exact analytical value of the geometric quantum discord for an arbitrary two-qudit state of any dimension via the parameters of its correlation matrix and the Bloch vectors of its reduced states. This general analytical result includes all the known exact results on the geometric quantum discord only as particular cases and proves rigorously that the lower bound on the geometric discord presented in [S. Rana *et al.*, Phys. Rev. A **85**, 024102 (2012)] constitutes its exact value for each two-qudit state. Moreover, our general result allows us to find for an arbitrary two-qudit state, pure or mixed, the upper and lower bounds on its geometric quantum discord, expressed via the Hilbert space characteristics of this state.

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I. INTRODUCTION

As shown by Bell theoretically [1] and later experimentally by Aspect *et al.* [2], the probabilistic description of a quantum correlation scenario does not, in general, agree with the classical probability model. Nonclassicality of quantum correlations is one of the main resources for many quantum information processing tasks. Among these quantum resources, Bell nonlocality and entanglement are the most studied; see [3–6] and references therein for the quantitative and qualitative relations between them.

Nevertheless, there are quantum states that exhibit nonclassical correlations even without entanglement and this led to the notion of the quantum discord [7], which is conceptually rich; however, it is very hard to calculate it even for a two-qubit state [8].

Due to the complexity [9] of computation of the quantum discord, there were also introduced related concepts, like the measurement-induced nonlocality [10] and the geometric quantum discord [11].

The geometric quantum discord is a geometric measure of quantum correlations of a bipartite quantum state, which is defined via the distance from this state to the set Ω of all states with the vanishing quantum discord [11]. In the present article, the geometric quantum discord $\mathcal{D}_g(\rho)$ of a two-qubit state ρ on $\mathcal{H}_{d_1} \otimes \mathcal{H}_{d_2}$ is defined via the Hilbert-Schmidt norm between states:

$$\mathcal{D}_g(\rho) := \min_{\chi \in \Omega} ||\rho - \chi||_2^2. \quad (1)$$

In other definitions [12–14] of the geometric quantum discord, different than in (1) distances are used.

Though the optimization problem for the computation of the geometric quantum discord of a bipartite state is much simpler than that for the quantum discord, its exact value has been explicitly computed only in some particular cases—namely, for a general two-qubit state [11], a general qubit-qudit state [15], a general pure two-qudit state [16], and some special families of mixed two-qudit states [15,17].

However, to our knowledge, for a general two-qudit state of an arbitrary dimension, the explicit exact analytical value of the geometric quantum discord has not been reported in the literature—only its lower bounds [15,17–20].

Geometric quantum discord is a useful concept with applications to quantum state discrimination [21], decoherence [22–25], quantum phase estimation, quantum teleportation, and remote state preparation protocols; see [26] and references therein. For certain states and certain quantum channels, geometric quantum discord has been shown [27–29] to be more resilient than entanglement in dissipative environments, making it a more robust measure for quantifying quantum correlations in decoherence scenarios. Recent studies suggest that geometric quantum discord is also a valuable quantification of quantum correlations in high-energy physics [30] and quantum gravity [31,32] contexts.

In the present paper, for an arbitrary two-qudit state ρ on $\mathcal{H}_{d_1} \otimes \mathcal{H}_{d_2}$, pure or mixed, we find in the explicit form the exact analytical value of its geometric quantum discord (1). This rigorously proved general result indicates that the lower bound on the geometric quantum discord found in [15] constitutes its exact value for each two-qudit state and includes only as particular cases the exact results for (i) general two-qubit [11] and qubit-qudit states [15], (ii) an arbitrary pure two-qudit state [16], and (iii) some special families of two-qudit states [15,17]. It also allows us to find the general upper bounds on the geometric quantum discord of an arbitrary two-qudit state in terms of its Hilbert space characteristics.

The paper is organized as follows. In Sec. II, we introduce the main issues of the general Bloch vectors formalism [33]

*Contact author: elena.loubenets@hse.ru

for a finite-dimensional quantum system on which we build up the calculations in this paper. In Sec. III, we find in the explicit analytical form the exact value of the geometric quantum discord for an arbitrary two-qudit state. In Sec. IV, this result allows us to find general upper and lower bounds on the geometric quantum discord in a general two-qudit case. In Sec. V, we discuss the main results of this paper and their importance for the practical tasks involving two-qudit quantum systems.

II. PRELIMINARIES: GENERAL BLOCH VECTORS FORMALISM

In this section, we briefly recall the main issues of the general Bloch vectors mathematical formalism developed in [33] for the description of properties and behavior of a finite-dimensional quantum system.

Consider the vector space $\mathcal{L}_d$ of all linear operators X on a complex Hilbert space $\mathcal{H}_d$ of a finite dimension $d \geqslant 2$. Equipped with the scalar product $\langle X_i, X_j\rangle_{\mathcal{L}_d} := \mathrm{tr}[X_i^\dagger X_j]$, $\mathcal{L}_d$ is a Hilbert space of the dimension d^2, referred to as Hilbert-Schmidt. Denote by

$$\begin{aligned}\mathfrak{B}_{\Upsilon_d} &:= \{\mathbb{I}_d,\ \Upsilon_d^{(j)} \in \mathcal{L}_d,\ \ j = 1,\dots,(d^2-1)\},\\ \Upsilon_d^{(j)} &= \big(\Upsilon_d^{(j)}\big)^\dagger \neq 0,\\ \mathrm{tr}\big[\Upsilon_d^{(j)}\big] &= 0, \quad \mathrm{tr}\big[\Upsilon_d^{(j)}\Upsilon_d^{(m)}\big] = 2\delta_{jm}\end{aligned} \tag{2}$$

an operator basis in $\mathcal{L}_d$ consisting of the identity operator $\mathbb{I}_d$ on $\mathcal{H}_d$ and a tuple $\Upsilon_d := (\Upsilon_d^{(1)},\dots,\Upsilon_d^{(d^2-1)})$ of traceless Hermitian operators mutually orthogonal in $\mathcal{L}_d$. For $d \geqslant 3$, some properties of a particular basis of this type, resulting in the generalized Gell-Mann representation, were considered in [34–42].

For an arbitrary qudit state ρ, the decomposition via a basis (2) constitutes the generalized Bloch representation [33]

$$\rho_d = \frac{\mathbb{I}_d}{d} + \sqrt{\frac{d-1}{2d}}(r_{\Upsilon_d}\cdot\Upsilon_d), \tag{3}$$

$$r_{\Upsilon_d}\cdot\Upsilon_d := \sum_{j=1}^{d^2-1} r_{\Upsilon_d}^{(j)}\Upsilon_d^{(j)}, \tag{4}$$

$$r_{\Upsilon_d} = \sqrt{\frac{d}{2(d-1)}}\ \mathrm{tr}[\rho_d\Upsilon_d] \in \mathbb{R}^{d^2-1}, \tag{5}$$

where $r_{\Upsilon_d} \in \mathbb{R}^{d^2-1}$ is referred to as the Bloch vector of a qudit state ρ_d. For a state ρ_d, the norm of its Bloch vector satisfies the relations

$$\|r_{\Upsilon_d}\|^2_{\mathbb{R}^{d^2-1}} = \frac{d}{d-1}\left(\mathrm{tr}\big[\rho_d^2\big] - \frac{1}{d}\right) \leqslant 1 \tag{6}$$

and is independent of the choice of a tuple Υ_d in an operator basis (2). For the maximally mixed state, the Bloch vector is equal to zero.

If a state ρ_d is pure, then the norm of its Bloch vector r_{Υ_d} is equal to $\|r_{\Upsilon_d}\|_{\mathbb{R}^{d^2-1}} = 1$. However, in contrast to a qubit case, for an arbitrary $d > 2$, not any unit vector $r \in \mathbb{R}^{d^2-1}$ corresponds via representation

$$\tau_d = \frac{\mathbb{I}_d}{d} + \sqrt{\frac{d-1}{2d}}(r\cdot\Upsilon_d) \tag{7}$$

to a pure state.

Namely, by Proposition 7 and Theorem 2 in [33] a Hermitian operator (7) with the unit trace constitutes a pure state if and only if

$$\|r\|^2_{\mathbb{R}^{d^2-1}} = 1, \quad \|(r\cdot\Upsilon_d)^{(-)}\|_0 = \sqrt{\frac{2}{d(d-1)}}, \tag{8}$$

where notation $\|\cdot\|_0$ means the operator norm of a linear operator on $\mathcal{H}_d$ and notation $X^{(-)}$ means the nonnegative operator in the unique decomposition of a self-adjoint operator X via $X = X^{(+)} - X^{(-)}$, where $X^{(\pm)} \geqslant 0$, $X^{(+)}X^{(-)} = X^{(-)}X^{(+)} = 0$.

For $d = 2$ and $\Upsilon_2 = \sigma = (\sigma_1, \sigma_2, \sigma_3)$, where σ is the qubit spin operator on $\mathbb{C}^2$, the first of the relations in (8) implies the second one.

From (3) and (6) it follows that, for a state ρ_d, the values of the norms $\|r_{\Upsilon_d}\|_{\mathbb{R}^{d^2-1}}$ and $\|(r_{\Upsilon_d}\cdot\Upsilon_d)^{(-)}\|_0$ do not depend on a choice of a tuple Υ_d in decomposition (3).

Note that, by Lemma 1 in [42], the bounds

$$\sqrt{\frac{2}{d}} \leqslant \frac{\|r\cdot\Upsilon_d\|_0}{\|r\|_{\mathbb{R}^{d^2-1}}} \leqslant \sqrt{\frac{2(d-1)}{d}} \tag{9}$$

hold for any vector $r \in \mathbb{R}^{d^2-1}$ and any tuple Υ_d .

By Eq. (70) in [33], for any two qudit states ρ_d, ρ_d', the scalar product of their Bloch vectors satisfies the relation

$$r_{\Upsilon_d}\cdot r'_{\Upsilon_d} \geqslant -\frac{1}{d-1}, \tag{10}$$

where equality holds iff $\mathrm{tr}[\rho_d\rho_d'] = 0$.

In view of Theorem 2 in [33], relation (10), and identity $\sum_k |k\rangle\langle k| = \mathbb{I}_d$, valid for any orthonormal basis $\{|k\rangle \in \mathcal{H}_d,\ k = 1,\dots,d\}$, we have the following statement needed for our proof of Theorem 1 in Sec. III.

Proposition 1. Representation (7) establishes the one-to-one correspondence between orthonormal bases $\{|k\rangle \in \mathcal{H}_d,\ k = 1,\dots,d\}$ in $\mathcal{H}_d$ and sets

$$\Omega_{\Upsilon_d} = \{y_k \in \mathbb{R}^{d^2-1},\ k = 1,\dots,d\} \tag{11}$$

of vectors y_k in $\mathbb{R}^{d^2-1}$, satisfying the relations

$$\sum_{k=1}^{d} y_k = 0, \quad \|y_k\|_{\mathbb{R}^{d^2-1}} = 1, \quad y_{k_1}\cdot y_{k_2} = -\frac{1}{d-1}, \quad \forall k_1 \neq k_2, \tag{12}$$

$$\|(y_k\cdot\Upsilon_d)^{(-)}\|_0 = \sqrt{\frac{2}{d(d-1)}}, \quad \forall k = 1,\dots,d. \tag{13}$$

For a two-qudit state $\rho_{d_1\times d_2}$ on $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}$, $d_1, d_2 \geqslant 2$, the representation

$$\begin{aligned}\rho_{d_1\times d_2} = {} & \frac{\mathbb{I}_{d_1}\otimes\mathbb{I}_{d_2}}{d_1 d_2} + \sqrt{\frac{d_1-1}{2d_1}}\,(r_1\cdot\Upsilon_{d_1})\otimes\frac{\mathbb{I}_{d_2}}{d_2}\\ &+ \sqrt{\frac{d_2-1}{2d_2}}\,\frac{\mathbb{I}_{d_1}}{d_1}\otimes\big(r_2\cdot\Upsilon_{d_2}\big)\\ &+ \frac{1}{4}\sum_{i,j} T^{(ij)}_{\rho_{d_1\times d_2}}\big(\Upsilon_{d_1}^{(i)}\otimes\Upsilon_{d_2}^{(j)}\big)\end{aligned} \tag{14}$$

is referred [33] to as the generalized Pauli representation and constitutes decomposition (3) via the operator basis of type (2) with the elements having the tensor product form

$$\mathbb{I}_{d_1}\otimes\mathbb{I}_{d_2},\quad \Upsilon_{d_1}^{(i)}\otimes\frac{\mathbb{I}_{d_2}}{\sqrt{d_2}},\quad \frac{\mathbb{I}_{d_1}}{\sqrt{d_1}}\otimes\Upsilon_{d_2}^{(j)},\quad \Upsilon_{d_1}^{(i)}\otimes\Upsilon_{d_2}^{(j)},$$
$$i=1,\dots,(d_1^2-1),\quad j=1,\dots,(d_2^2-1),$$
$$\Upsilon_{d_n}^{(m)}=\left(\Upsilon_{d_n}^{(m)}\right)^{\dagger}\neq 0,\quad \mathrm{tr}\left[\Upsilon_{d_n}^{(m)}\right]=0,$$
$$\mathrm{tr}\left[\Upsilon_{d_n}^{(m_1)}\Upsilon_{d_n}^{(m_2)}\right]=2\delta_{m_1m_2},\quad n=1,2. \tag{15}$$

In representation (14),

$$r_1=\sqrt{\frac{d_1}{2(d_1-1)}}\mathrm{tr}\left[\rho_{d_1\times d_2}\left(\Upsilon_{d_1}\otimes\mathbb{I}_{d_2}\right)\right]\in\mathbb{R}^{d_1^2-1}, \tag{16}$$
$$r_2=\sqrt{\frac{d_2}{2(d_2-1)}}\mathrm{tr}\left[\rho_{d_1\times d_2}\left(\mathbb{I}_{d_1}\otimes\Upsilon_{d_2}\right)\right]\in\mathbb{R}^{d_2^2-1},$$
$$\|r_1\|_{\mathbb{R}^{d_1^2-1}}\leqslant 1,\ \|r_2\|_{\mathbb{R}^{d_2^2-1}}\leqslant 1, \tag{17}$$

are the Bloch vectors of states $\rho_1=\mathrm{tr}_{\mathcal{H}_2}[\rho_{d_1\times d_2}]$ and $\rho_2=\mathrm{tr}_{\mathcal{H}_1}[\rho_{d_1\times d_2}]$ on $\mathcal{H}_{d_1}$ and $\mathcal{H}_{d_2}$, respectively, reduced from a two-qudit state $\rho_{d_1\times d_2}$ and satisfying the relation

$$\mathrm{tr}\left[\rho_j^2\right]=\frac{1}{d_j}+\frac{d_j-1}{d_j}||r_j||^2_{\mathbb{R}^{d_j^2-1}},\quad j=1,2, \tag{18}$$

while

$$T^{(ij)}_{\rho_{d_1\times d_2}}:=\mathrm{tr}\left[\rho_{d_1\times d_2}\left(\Upsilon_{d_1}^{(i)}\otimes\Upsilon_{d_2}^{(j)}\right)\right], \tag{19}$$
$$i=1,\dots,d_1^2-1,\quad j=1,\dots,d_2^2-1,$$

are the elements of the real-valued matrix $T_{\rho_{d_1\times d_2}}$ referred to as the correlation matrix of a two-qudit state $\rho_{d_1\times d_2}$.

In case of a pure two-qudit state $\rho_{d_1\times d_2}$, $d_1,d_2\geqslant 2$, by the Schmidt theorem $\mathrm{tr}[\rho_1^2]=\mathrm{tr}[\rho_2^2]$ and, in view of relation (18), this implies

$$\frac{1}{d_1}+\frac{d_1-1}{d_1}\|r_1\|^2_{\mathbb{R}^{d_1^2-1}}=\frac{1}{d_2}+\frac{d_2-1}{d_2}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}}. \tag{20}$$

From the generalized Pauli representation (14) it also follows that

$$\mathrm{tr}\left[\rho^2_{d_1\times d_2}\right]=\frac{1}{d_1d_2}+\frac{d_1-1}{d_1d_2}\|r_1\|^2_{\mathbb{R}^{d_1^2-1}}+\frac{d_2-1}{d_1d_2}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}}+\frac{1}{4}\sum_{i,j}\left(T^{(ij)}_{\rho_{d_1\times d_2}}\right)^2, \tag{21}$$

so that expression (21) and relation $\mathrm{tr}[\rho^2_{d_1\times d_2}]\leqslant 1$ imply

$$\frac{d_1-1}{d_1d_2}\|r_1\|^2_{\mathbb{R}^{d_1^2-1}}+\frac{d_2-1}{d_1d_2}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}}+\frac{1}{4}\sum_{i,j}\left(T^{(ij)}_{\rho_{d_1\times d_2}}\right)^2\leqslant\frac{d_1d_2-1}{d_1d_2}, \tag{22}$$

where equality holds iff a state $\rho_{d_1\times d_2}$ is pure.

Since in equality (21) the values of trace $\mathrm{tr}[\rho^2_{d_1\times d_2}]$ and the Bloch vectors' norms $\|r_1\|^2_{\mathbb{R}^{d_1^2-1}}$ and $\|r_2\|^2_{\mathbb{R}^{d_2^2-1}}$ do not depend on a choice of tuples Υ_{d_1}, Υ_{d_2} in decomposition (14), the same is true for the sum $\sum_{i,j}(T^{(ij)}_{\rho_{d_1\times d_2}})^2=\mathrm{tr}[T^{\dagger}_{\rho_{d_1\times d_2}}T_{\rho_{d_1\times d_2}}]$, which constitutes the trace of the positive operator $T^{\dagger}_{\rho_{d_1\times d_2}}T_{\rho_{d_1\times d_2}}$ on $\mathbb{R}^{d_2^2-1}$.

If $d_1=d_2=:d$, then, for every two-qudit state $\rho_{d\times d}$ on $\mathcal{H}_d\otimes\mathcal{H}_d$, $d\geqslant 2$,

$$\|r_1\|^2_{\mathbb{R}^{d^2-1}}+\|r_2\|^2_{\mathbb{R}^{d^2-1}}+\frac{d^2}{4(d-1)}\mathrm{tr}[T^{\dagger}_{\rho_{d\times d}}T_{\rho_{d\times d}}]\leqslant d+1, \tag{23}$$

and the bound (48) in [42] and the above upper bound in (9) imply

$$\|T_{\rho_{d\times d}}n\|^2_{\mathbb{R}^{d^2-1}}\leqslant\sqrt{\frac{2}{d}}\sqrt{\frac{2(d-1)}{d}}\|T_{\rho_{d\times d}}n\|_{\mathbb{R}^{d^2-1}}$$
$$\Rightarrow\|T_{\rho_{d\times d}}n\|_{\mathbb{R}^{d^2-1}}\leqslant 2\frac{\sqrt{d-1}}{d}, \tag{24}$$

for all $n\in\mathbb{R}^{d^2-1}$, $\|n\|\leqslant\frac{1}{\sqrt{d-1}}$. This implies that, for every two-qudit state and any tuples Υ_{d_1}, Υ_{d_2}, the spectral (operator) norm $\|T\|_0$ of the correlation matrix T is upper bounded by

$$\|T_{\rho_{d\times d}}\|_0:=\sup_{\|n\|=1}\|T_{\rho_{d\times d}}n\|_{\mathbb{R}^{d^2-1}}$$
$$=\sqrt{d-1}\sup_{\|n\|=1}\left\|T_{\rho_{d\times d}}\left(\frac{n}{\sqrt{d-1}}\right)\right\|_{\mathbb{R}^{d^2-1}}$$
$$\leqslant\frac{2(d-1)}{d}. \tag{25}$$

Recall that $\|T_{\rho_{d\times d}}\|_0^2$ is the maximal eigenvalue of the positive self-adjoint operator $T^{\dagger}_{\rho_{d\times d}}T_{\rho_{d\times d}}$.

Furthermore, for every separable two-qudit state

$$\rho^{(sep)}_{d\times d}=\sum_k\beta_k\rho_1^{(k)}\otimes\rho_2^{(k)},\quad\beta_k>0,\quad\sum_k\beta_k=1, \tag{26}$$

on $\mathcal{H}_d\otimes\mathcal{H}_d$, $d\geqslant 2$, the correlation matrix $T_{\rho^{(sep)}_{d\times d}}$ and the Bloch vectors (16), (17) have the form

$$T_{\rho^{(sep)}_{d\times d}}=\frac{2(d-1)}{d}\sum_k\beta_k\left|r_1^{(k)}\right\rangle\!\left\langle r_2^{(k)}\right|,$$
$$r_1=\sum_k\beta_kr_1^{(k)},\quad r_2=\sum_k\beta_kr_2^{(k)}, \tag{27}$$

where $r_j^{(k)}$ are the Bloch vectors of states $\rho_j^{(k)}$, $j=1,2$, given by (5), and the operator norm of the correlation matrix is upper bounded by

$$\left\|T_{\rho^{(sep)}_{d\times d}}\right\|_0\leqslant\frac{2(d-1)}{d}\sum_k\beta_k\left\|\left|r_1^{(k)}\right\rangle\!\left\langle r_2^{(k)}\right|\right\|_0$$
$$=\frac{2(d-1)}{d}\sum_k\beta_k\left\|r_1^{(k)}\right\|_{\mathbb{R}^{d^2-1}}\left\|r_2^{(k)}\right\|_{\mathbb{R}^{d^2-1}}$$
$$\leqslant\frac{2(d-1)}{d}. \tag{28}$$

The concurrence $\mathrm{C}_{|\psi\rangle\langle\psi|}$ of a pure two-qudit state $\rho_{d_1\times d_2}=|\psi\rangle\langle\psi|$ on $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}$, $d_1,d_2\geqslant 2$, is defined by the relation

$$\mathrm{C}_{|\psi\rangle\langle\psi|}=\sqrt{2\left(1-\mathrm{tr}\left[\rho_j^2\right]\right)} \tag{29}$$

and, in view of Eqs. (18) and (20), takes the form

$$\mathrm{C}_{|\psi\rangle\langle\psi|} = \sqrt{2\frac{d_i-1}{d_j}\left(1-\|r_j\|^2_{\mathbb{R}^{d_j^2-1}}\right)}, \quad j=1,2. \tag{30}$$

If we introduce the concurrence $\widetilde{\mathrm{C}}_{|\psi\rangle\langle\psi|}$ normalized to unity in the case of a maximally entangled quantum state, as it is done in [33], then

$$\mathrm{C}_{|\psi\rangle\langle\psi|} = \sqrt{2\frac{d_k-1}{d_k}}\widetilde{\mathrm{C}}_{|\psi\rangle\langle\psi|}, \quad d_k = \min\{d_1,d_2\}, \tag{31}$$

and

$$\widetilde{\mathrm{C}}_{|\psi\rangle\langle\psi|} = \sqrt{1-\|r_k\|^2_{\mathbb{R}^{d_k^2-1}}}. \tag{32}$$

In a two-qubit case, $\widetilde{\mathrm{C}}_{|\psi\rangle\langle\psi|} = \mathrm{C}_{|\psi\rangle\langle\psi|}$.

For a general state $\rho_{d_1\times d_2}$, pure or mixed, concurrence C_ρ is defined via the relation

$$\mathrm{C}_{\rho_{d_1\times d_2}} = \inf_{\{\alpha_i,\psi_i\}}\sum \alpha_i \mathrm{C}_{|\psi_i\rangle\langle\psi_i|}, \tag{33}$$

where $\rho_{d_1\times d_2} = \sum_i \alpha_i|\psi_i\rangle\langle\psi_i|$, $\sum_i\alpha_i = 1$, $\alpha_i > 0$ is a possible convex decomposition of the state $\rho_{d_1\times d_2}$ via pure states; see [5,43] and references therein.

III. GEOMETRIC QUANTUM DISCORD

A general quantum-classical[1]. state on $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}$ has the form

$$\chi_{d_1\times d_2} = \sum_{k=1}^{d_2}\alpha_k\sigma_k\otimes|k\rangle\langle k|, \quad \alpha_k\geqslant 0, \quad \sum_k\alpha_k = 1,$$
$$|k\rangle\in\mathcal{H}_{d_2}, \quad k=1,\dots,d_2, \quad \langle k_{j_1}|k_{j_2}\rangle = \delta_{j_1j_2},$$
$$\sum_{k=1}^{d_2}|k\rangle\langle k| = \mathbb{I}_{d_2}. \tag{34}$$

For short, we further omit the below indices at states indicating its dimensions at two sites.

In order to find the geometric quantum discord $\mathcal{D}_g(\rho) := \min_\chi \mathrm{tr}[(\rho-\chi)^2]$ of a state ρ, let us consider the decomposition of the difference between states ρ and χ via their generalized Pauli representations (14). We have

[1]In this paper, we refer to the right geometric discord instead of the left discord as in [11]

$$\rho-\chi = \sqrt{\frac{d_1-1}{2d_1}}\left[\left(r_1-\sum_{k=1}^{d_2}\alpha_k x_k\right)\cdot\Upsilon_{d_1}\right]\otimes\frac{\mathbb{I}_{d_2}}{d_2} + \sqrt{\frac{d_2-1}{2d_2}}\frac{\mathbb{I}_{d_1}}{d_1}\otimes\left[\left(r_2-\sum_{k=1}^{d_2}\alpha_k y_k\right)\cdot\Upsilon_{d_2}\right]$$
$$+\frac{1}{4}\sum_{\substack{i=1,\dots,d_1,\\ j=1,\dots,d_2}}\left(T_\rho^{(ij)} - 2\sqrt{\frac{(d_1-1)(d_2-1)}{d_1d_2}}\sum_{k=1}^{d_2}\alpha_k x_k^{(i)}y_k^{(j)}\right)\Upsilon_{d_1}^{(i)}\otimes\Upsilon_{d_2}^{(j)}, \tag{35}$$

where the Bloch vectors $r_1\in\mathbb{R}^{d_1^2-1}$, $r_2\in\mathbb{R}^{d_2^2-1}$ and $T_\rho^{(ij)}$ are defined in (16), (17), and (19), respectively, and have norms $\|r_1\|_{\mathbb{R}^{d_1^2-1}}\leqslant 1$, $\|r_2\|_{\mathbb{R}^{d_2^2-1}}\leqslant 1$, whereas for $k=1,\dots,d_2$,

$$x_k = \sqrt{\frac{d_1}{2(d_1-1)}}\mathrm{tr}[\sigma_k\Upsilon_{d_1}]\in\mathbb{R}^{d_1^2-1}, \quad \|x_k\|_{\mathbb{R}^{d_1^2-1}}\leqslant 1,$$
$$y_k = \sqrt{\frac{d_2}{2(d_2-1)}}\langle k|\Upsilon_{d_2}|k\rangle\in\mathbb{R}^{d_2^2-1}, \quad \|y_k\|_{\mathbb{R}^{d_2^2-1}} = 1 \tag{36}$$

are, respectively, the Bloch vectors of states σ_k on $\mathcal{H}_{d_1}$ and mutually orthogonal pure states $|k\rangle\langle k|$, $\sum_{k=1}^{d_2}|k\rangle\langle k| = \mathbb{I}_{d_2}$, on $\mathcal{H}_{d_2}$.

By Proposition 1, representation (7) establishes the one-to-one correspondence between orthonormal bases in $\mathcal{H}_{d_2}$ and sets $\Omega_{\Upsilon_{d_2}} = \{y_k\in\mathbb{R}^{d_2^2-1},\ k=1,\dots,d_2\}$ of vectors in $\mathbb{R}^{d_2^2-1}$, satisfying the relations

$$\sum_{k=1}^{d_2}y_k = 0, \quad \|y_k\|_{\mathbb{R}^{d_2^2-1}} = 1, \quad y_{k_1}\cdot y_{k_2} = -\frac{1}{d_2-1}, \tag{37}$$
$$\forall k_1\neq k_2,$$
$$\left\|\left(y_k\cdot\Upsilon_{d_2}\right)^{(-)}\right\|_0 = \sqrt{\frac{2}{d_2(d_2-1)}}, \quad \forall k=1,\dots,d_2. \tag{38}$$

Equation (35) implies

$$\mathrm{tr}[(\rho-\chi)^2] = \frac{d_1-1}{d_1d_2}\left\|r_1-\sum_{k=1}^{d_2}\alpha_k x_k\right\|^2_{\mathbb{R}^{d_1^2-1}} + \frac{d_2-1}{d_1d_2}\left\|r_2-\sum_{k=1}^{d_2}\alpha_k y_k\right\|^2_{\mathbb{R}^{d_2^2-1}}$$
$$+\frac{1}{4}\sum_{i,j}\left(T_\rho^{(ij)} - 2\sqrt{\frac{(d_1-1)(d_2-1)}{d_1d_2}}\sum_{k=1}^{d_2}\alpha_k x_k^{(i)}y_k^{(j)}\right)^2 \tag{39}$$

and, under conditions (37), relation (39) reduces to

$$\mathrm{tr}[(\rho-\chi)^2] = \frac{d_2-1}{d_1 d_2}\|r_2\|^2_{\mathbb{R}^{d^2-1}} + \frac{1}{4}\mathrm{tr}[T_\rho^\dagger T_\rho] + \frac{d_1-1}{d_1}\sum_{k=1}^{d_2}\left\|\alpha_k x_k - \frac{r_1}{d_2} - \frac{1}{2}\sqrt{\frac{d_1(d_2-1)}{d_2(d_1-1)}}T_\rho y_k\right\|^2_{\mathbb{R}^{d_1^2-1}}$$
$$+\frac{1}{d_1}\sum_{k=1}^{d_2}\left[\alpha_k - \frac{1}{d_2} - \frac{d_2-1}{d_2}(r_2\cdot y_k)\right]^2 - \frac{(d_2-1)^2}{d_2^2 d_1}\sum_{k=1}^{d_2}(r_2\cdot y_k)^2 - \frac{d_2-1}{4d_2}\sum_{k=1}^{d_2}\|T_\rho y_k\|^2_{\mathbb{R}^{d_1^2-1}}. \quad (40)$$

From relation (40) it follows that, for a fixed set $\{y_k\}$, the minimum of $\mathrm{tr}[(\rho-\chi)^2]$ over x_k and α_k is attained at

$$\alpha_k x_k = \frac{r_1}{d_2} - \frac{1}{2}\sqrt{\frac{d_1(d_2-1)}{d_2(d_1-1)}}T_\rho y_k,$$
$$\alpha_k = \frac{1}{d_2} + \frac{d_2-1}{d_2}(r_2\cdot y_k) \Rightarrow \sum_{k=1}^{d_2}\alpha_k = 1, \quad (41)$$

such that

$$\left\|\frac{r_1}{d_2} - \frac{1}{2}\sqrt{\frac{d_1(d_2-1)}{d_2(d_1-1)}}T_\rho y_k\right\|_{\mathbb{R}^{d_1^2-1}} \leqslant 1. \quad (42)$$

Taking this into account in relation (40), we come to the following statement.

Proposition 2. For every two-qudit state ρ on $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}$, the geometric quantum discord $\mathcal{D}_g(\rho) = \min_\chi \mathrm{tr}[(\rho-\chi)^2]$ is given by

$$\mathcal{D}_g(\rho) = \frac{d_2-1}{d_1 d_2}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}} + \frac{1}{4}\mathrm{tr}[T_\rho^\dagger T_\rho] - \max_{\Omega_{\Upsilon_{d_2}}}\mathrm{tr}\left[\left(\frac{d_2-1}{d_1 d_2}|r_2\rangle\langle r_2| \;+\; \frac{1}{4}T_\rho^\dagger T_\rho\right)\Pi_{\Omega_{\Upsilon_{d_2}}}\right], \quad (43)$$

where (i) T_ρ is the correlation matrix (19) of a state ρ and r_2 is the Bloch vector (17) of the reduced state $\rho_2 = \mathrm{tr}_{\mathcal{H}_1}[\rho]$ on $\mathcal{H}_{d_2}$ within decomposition (14) specified with arbitrary tuples Υ_{d_1} and Υ_{d_2} and (ii) the positive Hermitian operator $\Pi_{\Omega_{\Upsilon_{d_2}}}$ on $\mathbb{R}^{d_2^2-1}$ is defined by the relation

$$\Pi_{\Omega_{\Upsilon_{d_2}}} := \frac{d_2-1}{d_2}\sum_{k=1}^{d_2}|y_k\rangle\langle y_k|, \quad (44)$$

where

$$\Omega_{\Upsilon_{d_2}} = \left\{y_k\in\mathbb{R}^{d_2^2-1},\ k=1,\dots,d_2\right\}\subset\mathbb{R}^{d_2^2-1} \quad (45)$$

is a set of linear dependent vectors in $\mathbb{R}^{d_2^2-1}$, satisfying relations (37) and (38). In (43), notations $|r_2\rangle$ and $\langle r_2|$ mean the column vector and the line vector, corresponding to tuple $r_2 = (r_2^{(1)},\dots,r_2^{(d_2^2-1)})\in\mathbb{R}^{d_2^2-1}$.

The following statement is proved in the Appendix.

Lemma 1. For any tuple Υ_{d_2}, a positive operator (44) on $\mathbb{R}^{d_2^2-1}$ is an orthogonal projection of rank (d_2-1).

Taking into account Proposition 2 and Lemma 1, we proceed to introduce for a two-qudit state ρ, pure or mixed and of any dimension, the explicit exact analytical value of its geometric quantum discord $\mathcal{D}_g(\rho)$ in terms of characteristics of this state within the generalized Pauli representation (14).

Theorem 1. For an arbitrary two-qudit state ρ on $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}$, $d_1, d_2\geqslant 2$, the geometric quantum discord is equal to

$$\mathcal{D}_g(\rho) = \frac{d_2-1}{d_1 d_2}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}} + \frac{1}{4}\mathrm{tr}[T_\rho^\dagger T_\rho] - \sum_{n=1}^{d_2-1}\eta_n = \sum_{n=d_2}^{d_2^2-1}\eta_n, \quad (46)$$

where $\eta_1\geqslant\eta_2\geqslant\cdots\geqslant\eta_{d_2^2-1}\geqslant 0$ are the eigenvalues of the positive Hermitian operator

$$G(\rho) = \frac{d_2-1}{d_1 d_2}|r_2\rangle\langle r_2| \;+\; \frac{1}{4}T_\rho^\dagger T_\rho \quad (47)$$

on $\mathbb{R}^{d_2^2-1}$ listed in decreasing order with the corresponding algebraic multiplicities. The eigenvalues of the positive operator $G(\rho)$ and the values of the norm $\|r_2\|^2_{\mathbb{R}^{d_2^2-1}}$ and the trace $\mathrm{tr}[T_\rho^\dagger T_\rho]$ are independent on a choice of tuples Υ_{d_1} and Υ_{d_2} within representation (14).

Proof. Let the Bloch vector $r_2\in\mathbb{R}^{d_2^2-1}$ and the correlation matrix T_ρ in (43) be defined within decomposition (14) for some arbitrary tuples Υ_{d_1} and Υ_{d_2}. As indicated in Sec. II, the values of the norm $\|r_2\|^2_{\mathbb{R}^{d_2^2-1}}\leqslant 1$ and the trace $\mathrm{tr}[T_\rho^\dagger T_\rho]$ do not depend on a choice of tuples Υ_{d_1} and Υ_{d_2} and are determined only by a state ρ . By Lemma 1 every positive operator $\Pi_{\Omega_{\Upsilon_{d_2}}}$, given by (44), is an orthogonal projection of rank (d_2-1), so that it has eigenvalue 1 of multiplicity (d_2-1) and the eigenvalue 0 with multiplicity $d_2(d_2-1)$. This and the von Neumann inequality [44] $\mathrm{tr}[AB]\leqslant\sum a_i b_i$, which is valid for any two positive operators A and B, with eigenvalues $a_i\geqslant 0$ and $b_i\geqslant 0$, listed in decreasing order, imply that, for each $\Pi_{\Omega_{\Upsilon_{d_2}}}$, the trace $\mathrm{tr}[G(\rho)\Pi_{\Omega_{\Upsilon_{d_2}}}]$, standing under the maximum in (43), is upper bounded by

$$\mathrm{tr}\left[G(\rho)\Pi_{\Omega_{\Upsilon_{d_2}}}\right]\leqslant\sum_{k=1}^{d_2-1}\eta_k. \quad (48)$$

Therefore, in order to prove the exact analytical expression (46), we have to present some projection $\Pi'_{\Omega_{\Upsilon_{d_2}}}$ on which the upper bound (48) is attained.

Let us introduce projections $\Pi_{\Omega_{\widetilde{\Upsilon}_{d_2}}} = \frac{d_2-1}{d_2}\sum_{k=1}^{d_2}|y_k\rangle\langle y_k|$, which are defined via vectors $y_k\in\Omega_{\widetilde{\Upsilon}_{d_2}}$ satisfying relations (37) and the condition (38), specified for some tuple $\widetilde{\Upsilon}_{d_2}\neq\Upsilon_{d_2}$, which we choose below. Let

$$\widetilde{\Upsilon}_{d_2}^{(j)} = \mathrm{v}_j\cdot\Upsilon_{d_2},\quad j=1,\dots,(d_2^2-1), \quad (49)$$

be the decomposition of traceless Hermitian operators $\widetilde{\Upsilon}_{d_2}^{(j)}$—elements of a tuple $\widetilde{\Upsilon}_{d_2}$—in the basis (2) specified with tuple Υ_{d_2}. The set of vectors $\{\mathrm{v}_j \in \mathbb{R}^{d_2^2-1},\ j = 1,\dots,(d_2^2-1)\}$ constitutes an orthonormal basis; see Eq. 18 in [33].

For a given projection

$$\widetilde{\Pi}_{\widetilde{\Omega}_{\widetilde{\Upsilon}_{d_2}}} = \frac{d_2-1}{d_2}\sum_{k=1}^{d_2} |\widetilde{y}_k\rangle\langle\widetilde{y}_k|, \quad k = 1,\dots,d_2, \tag{50}$$

denote by $\widetilde{g}_m$, $m = 1,\dots,d_2^2-1$, its mutually orthogonal eigenvectors, where the first (d_2-1) eigenvectors correspond to eigenvalue 1 and others to the eigenvalue 0. By the spectral theorem, we have

$$G(\rho) = \sum_{n=1}^{d_2^2-1} \eta_n |e_n\rangle\langle e_n|, \quad \widetilde{\Pi}_{\widetilde{\Omega}_{\widetilde{\Upsilon}_{d_2}}} = \sum_{m=1}^{d_2-1} |\widetilde{g}_m\rangle\langle\widetilde{g}_m|. \tag{51}$$

To projection (50) define via the unitary operator $\mathrm{U} = \sum_n |e_n\rangle\langle\widetilde{g}_n|$ the projection

$$\mathrm{U}\widetilde{\Pi}_{\widetilde{\Omega}_{\widetilde{\Upsilon}_{d_2}}}\mathrm{U}^\dagger = \frac{d_2-1}{d_2}\sum_{k=1}^{d_2} |y'_k\rangle\langle y'_k| = \sum_{n=1}^{d_2-1} |e_n\rangle\langle e_n|, \tag{52}$$

where vectors $y'_k = \mathrm{U}\widetilde{y}_k \in \mathbb{R}^{d_2^2-1}$ satisfy relations (37) and also relation (38)

$$\sqrt{\frac{2}{d_2(d_2-1)}} = \big\|\big(\widetilde{y}_k\cdot\widetilde{\Upsilon}_{d_2}\big)^{(-)}\big\|_0 = \big\|\big(y'_k\cdot\widetilde{\Upsilon}'_{d_2}\big)^{(-)}\big\|_0, \tag{53}$$

but with respect to tuple $\widetilde{\Upsilon}'_{d_2}$ with elements

$$\big(\widetilde{\Upsilon}'_{d_2}\big)^{(m)} = \sum_l \mathrm{U}^\dagger_{lm}\widetilde{\Upsilon}^{(l)}_{d_2}. \tag{54}$$

Substituting (49) into (54), we derive

$$\big(\widetilde{\Upsilon}'_{d_2}\big)^{(m)} = \sum_j \left(\sum_l \mathrm{U}^\dagger_{lm}\mathrm{v}^{(j)}_l\right)\Upsilon^{(j)}_{d_2}. \tag{55}$$

Choosing in (49) the orthonormal basis $\{\mathrm{v}_l \in \mathbb{R}^{d_2^2-1},\ l = 1,\dots,(d_2^2-1)\}$ with components $\mathrm{v}^{(j)}_l = \mathrm{U}_{jl}$, we have

$$\sum_l \mathrm{U}^\dagger_{lm}\mathrm{v}^{(j)}_l = \sum_l \mathrm{U}_{jl}\mathrm{U}^\dagger_{lm} = \delta_{jm} \Rightarrow \widetilde{\Upsilon}'_{d_2} = \Upsilon_{d_2}. \tag{56}$$

Therefore, under the above unitary transform of projection (50) and the specific choice via (49) of a tuple $\widetilde{\Upsilon}_{d_2}$ in (50), we come to the projection

$$\mathrm{U}\,\widetilde{\Pi}_{\Omega_{\widetilde{\Upsilon}_{d_2}}}\mathrm{U}^\dagger = \frac{d_2-1}{d_2}\sum_{k=1}^{d_2} |y_k\rangle\langle y_k| = \Pi'_{\Omega_{\Upsilon_{d_2}}}, \tag{57}$$

which is included into the set of projections over which the maximum in (43) is considered. Taking into account that, by relation (52), $\Pi'_{\Omega_{\Upsilon_{d_2}}} = \sum_{n=1}^{d_2-1}|e_n\rangle\langle e_n|$ we have[2]

$$\mathrm{tr}\big[G(\rho)\Pi'_{\Omega_{\Upsilon_{d_2}}}\big] = \mathrm{tr}\left[\sum_{n=1}^{d_2^2-1}\eta_n|e_n\rangle\langle e_n| \sum_{m=1}^{d_2-1}|e_m\rangle\langle e_m|\right] = \sum_{n=1}^{d_2-1}\eta_n. \tag{58}$$

Equations (48) and (58) prove the statement. ■

The general exact result (46) proved by Theorem 1 indicates that the lower bound on the geometric quantum discord presented in [15] is attained on every two-qudit state. Moreover, this exact result on the geometric quantum discord includes only as particular cases all the exact expressions known [11,15] for some particular mixed states.

We note that, in contrast to the derivation of the lower bound in [15] via the Pauli decomposition with the generalized Gell-Mann operators, our derivation of the exact value (46) is based on the Pauli decomposition with respect to any operator basis of the form (15). Also, the normalization coefficients in (46) are different from those in [15] and satisfy the general relations derived in [33] and presented briefly in Sec. II.

The following statement shows that, in the case of a pure two-qudit state, the exact general result (46) in Theorem 1 includes as a particular case the expression [16] for the geometric quantum discord of a pure two-qudit state, which was derived in [16] directly from the definition (1).

Corollary 1. For every pure two-qudit state $\rho_\psi = |\psi\rangle\langle\psi|$ on $\mathcal{H}_d \otimes \mathcal{H}_d$, $d \geqslant 2$, the geometric quantum discord is given by

$$\mathcal{D}_g(\rho_\psi) = \tfrac{1}{2}\mathrm{C}^2_{\rho_\psi} \leqslant 2\mathcal{N}^2_{\rho_\psi}, \tag{59}$$

where the equality in the right-hand side holds for a pure two-qubit state. Here, C_{ρ_ψ} is the concurrence (29) of a pure two-qudit state ρ_ψ and $\mathcal{N}_{\rho_\psi}$ is its negativity.[3] For a maximally entangled pure two-qudit state $\rho_{\psi_{\max}}$,

$$\mathcal{D}_g(\rho_{\psi_{\max}}) = \frac{d-1}{d}. \tag{60}$$

Proof. Consider first the geometric quantum discord for a pure two-qubit state. As it is found in Theorem 2 of [6], for a pure two-qubit state, the eigenvalues of the positive operator $T^\dagger_{\rho_\psi}T_{\rho_\psi}$ are equal to 1, $\mathrm{C}^2_{\rho_\psi}$, $\mathrm{C}^2_{\rho_\psi}$ and if $\|r_2\|^2_{\mathbb{R}^3} = 1 - \mathrm{C}^2_{\rho_\psi} \neq 0$ (that is, a pure state $|\psi\rangle$ is not maximally entangled), then the Bloch vector $r_2 \in \mathbb{R}^3$ constitutes [6] the eigenvector of matrix $T^\dagger_{\rho_\psi}T_{\rho_\psi}$. Therefore, if a pure two-qubit state $|\psi\rangle$ is not maximally entangled, then, in view of the spectral theorem,

[2]For our further consideration in Sec. IV, based on the proof of Theorem 1, we also formulate in Proposition 4 of the Appendix the general statement on $\max_{\Omega_y}\mathrm{tr}[A\Pi_{\Omega_y}]$ for any positive Hermitian operator A on $\mathbb{R}^{d^2-1}$.

[3]For a pure two-qudit state, the negativity takes the form $\sum_{1\leqslant k<m\leqslant d}\sqrt{\mu_k\mu_m}$; see, for example, Sec. 4 of [45].

the positive operator $G(\rho_\psi)$ in (47) takes the form

$$G(\rho_\psi) = \frac{1}{4}|r_2\rangle\langle r_2| + \frac{1}{4}\frac{|r_2\rangle\langle r_2|}{\|r_2\|^2_{\mathbb{R}^3}} + \frac{1}{4}\mathrm{C}^2_{\rho_\psi}(|\mathrm{v}_1\rangle\langle \mathrm{v}_1| + |\mathrm{v}_2\rangle\langle \mathrm{v}_2|)$$
$$= \frac{1}{4}\left(\|r_2\|^2_{\mathbb{R}^3}+1\right)\frac{|r_2\rangle\langle r_2|}{\|r_2\|^2_{\mathbb{R}^3}}+\frac{1}{4}\mathrm{C}^2_{\rho_\psi}(|\mathrm{v}_1\rangle\langle \mathrm{v}_1|+|\mathrm{v}_2\rangle\langle \mathrm{v}_2|), \tag{61}$$

where $|\mathrm{v}_1\rangle$, $|\mathrm{v}_2\rangle$ are two mutually orthogonal eigenvectors of $T^\dagger_{\rho_\psi}T_{\rho_\psi}$ corresponding to the eigenvalue $\mathrm{C}^2_{\rho_\psi}$ with multiplicity 2. Representation (61) implies that the eigenvalues of $G(\rho_\psi)$ are equal to

$$\eta_1 = \frac{1+\|r_2\|^2_{\mathbb{R}^3}}{4}, \quad \eta_{2,3} = \frac{\mathrm{C}^2_{\rho_\psi}}{4}. \tag{62}$$

For a maximally entangled two-qubit state $|\psi_{\max}\rangle$, the Bloch vector $r_2 = 0$, $T^\dagger_{\rho_{\psi_{\max}}}T_{\rho_{\psi\,\max}} = \mathbb{I}_{\mathbb{R}^3}$, and $G(\rho_{\psi_{\max}}) = \frac{1}{4}\mathbb{I}_{\mathbb{R}^3}$. Thus, for any pure two-qubit state $|\psi\rangle$, by (46) we have

$$\mathcal{D}_g(\rho_\psi) = \sum_{n=2}^{3}\eta_n = \frac{1}{2}\mathrm{C}^2_{\rho_\psi}. \tag{63}$$

The value of the geometric quantum discord of a two-qubit state via its negativity $\mathcal{N}_{\rho_\psi}$ follows from (63) and relation $\mathrm{C}_{\rho_\psi} = 2\mathcal{N}_{\rho_\psi}$ valid for every pure two-qubit state.

Let $d > 2$. Recall that, for any pure two-qudit state $|\psi\rangle\langle\psi|$ on $\mathcal{H}_d\otimes\mathcal{H}_d$, the nonzero eigenvalues $0 < \mu_k(\psi) \leqslant 1$ of its reduced states coincide and have the same multiplicity and vector $|\psi\rangle \in \mathcal{H}_d\otimes\mathcal{H}_d$ admits the Schmidt decomposition

$$|\psi\rangle = \sum_{1\leqslant n\leqslant r^{(\psi)}_{\mathrm{Sch}}}\sqrt{\mu_n(\psi)}\,\big|e^{(1)}_n\big\rangle\otimes\big|e^{(2)}_n\big\rangle, \qquad \sum_{1\leqslant n\leqslant r^{(\psi)}_{\mathrm{Sch}}}\mu_n(\psi)=1, \tag{64}$$

where $\mu_1 \geqslant \mu_2 \geqslant \cdots \geqslant \mu_{r^{(\psi)}_{\mathrm{Sch}}} > 0$ are nonzero eigenvalues of the reduced states of ρ_ψ, listed in the decreasing order and according to their multiplicity, and $\{|e^{(j)}_k\rangle \in \mathcal{H}\}$, $j = 1, 2$, are sets of the corresponding mutually orthogonal unit eigenvectors of the reduced states. Parameters $\sqrt{\mu_n(\psi)}$ and $1 \leqslant r^{(\psi)}_{\mathrm{Sch}} \leqslant d$ are called the Schmidt coefficients and the Schmidt rank of $|\psi\rangle$, respectively. For simplicity of further calculations, we present the decomposition (65) in the form

$$|\psi\rangle = \sum_{1\leqslant n\leqslant d}\sqrt{\mu_n(\psi)}\,\big|e^{(1)}_n\big\rangle\otimes\big|e^{(2)}_n\big\rangle \tag{65}$$

by adding into the sum the zero eigenvalues μ_n of the reduced states if $n > r^{(\psi)}_{\mathrm{Sch}}$.

As it is underlined in Theorem 1, the eigenvalues η_n of the positive operator $G(\rho)$, given by (47), are independent on a choice of tuples Υ_{d_1} and Υ_{d_2} in representation (14). Therefore, in the case of a pure two-qudit state ρ_ψ, for finding in expression (46) the sum $\sum_{n=d_2}^{d_2^2-1}\eta_n$ of the eigenvalues of $G(\rho_\psi)$, we take on each of the Hilbert spaces in $\mathcal{H}_d\otimes\mathcal{H}_d$ the tuple Υ_d of operators, which are similar by their structure to the generalized Gell-Mann operators presented by relations (4)–(6) in [42] but expressed not via the elements of the standard basis in $\mathbb{C}^d$ but via the elements of the corresponding orthonormal basis $\{|e^{(j)}_k\rangle \in \mathcal{H}_d\}$, $j = 1, 2$, in (65).

Under this choice, by relations (16), (17), (19), and (65) we find (quite similarly as it is done in Sec. 4 of [42]) that the matrix representation of the operator $G(\rho_\psi)$ is block-diagonal with the eigenvalues η_n for $n \geqslant d$ equal to $\mu_k\mu_m$, $1 \leqslant k < m \leqslant d$, each with multiplicity 2. Therefore, in (46)

$$\sum_{n=d_2}^{d_2^2-1}\eta_n = 2\sum_{1\leqslant k<m\leqslant d}\mu_k\mu_m. \tag{66}$$

This and the relation

$$\mathrm{C}^2_{\rho_\psi} = 2\left(1-\mathrm{tr}\left[\rho_j^2\right]\right) = 4\sum_{1\leqslant k<m\leqslant d}\mu_k\mu_m, \tag{67}$$

following from (29) and (65), prove the equality in (59). The upper bound in (59) follows[4] from the relation $C^2_{\rho_\psi} \leqslant 4(\sum_{1\leqslant k<m\leqslant d}\sqrt{\mu_k\mu_m})^2 = 4\mathcal{N}^2_{\rho_\psi}$, valid for any two-qudit state.

For a maximally entangled pure two-qudit state $\rho_{\psi_{\max}}$, the concurrence is equal to $\frac{2(d-1)}{d}$ and by (59) this implies (60). The latter relation follows also directly from (46), since, for a maximally entangled two-qudit state $\rho_{\psi_{\max}}$, the Bloch vector $r_2 = 0$, and the correlation matrix is diagonal [42] with all its singular values equal to $\frac{2}{d}$. Therefore,

$$G(\rho_{\psi_{\max}}) = \frac{1}{4}T^\dagger_{\rho_{\psi_{\max}}}T_{\rho_{\psi_{\max}}}, \quad \eta_n = \frac{1}{d^2}, \tag{68}$$

and, in view of (46), this implies

$$\mathcal{D}_g(\rho_{\psi_{\max}}) = \sum_{n=d}^{d^2-1}\eta_n = \frac{d(d-1)}{d^2} = \frac{d-1}{d}, \tag{69}$$

i.e., expression (60). ■

IV. UPPER AND LOWER BOUNDS

In this section, based on the result of Theorem 1, we introduce the general upper and lower bounds valid for an arbitrary two-qudit state and also specify the upper bound in the case of a separable two-qudit state.

Theorem 2. For an arbitrary two-qudit state ρ, pure or mixed, on $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}$, $d_1, d_2 \geqslant 2$, its geometric quantum discord admits the following upper bounds:

$$\mathcal{D}_g(\rho) \leqslant \frac{d_2-1}{d_2}\left[1-\frac{\|r_2\|^2}{d_2+1}\right] \tag{70}$$
$$\leqslant \frac{d_2-1}{d_2}, \tag{71}$$

where the upper bound (71) constitutes the geometric discord of the maximally entangled two-qudit state if $\min\{d_1, d_2\} = d_2$.

Proof. Taking into account that

$$\mathrm{tr}[G(\rho)] = \sum_{n=1}^{d_2^2-1}\eta_n = \frac{d_2-1}{d_2d_1}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}} + \frac{1}{4}\mathrm{tr}[T^\dagger_\rho T_\rho] \tag{72}$$

[4] For the expression of the negativity of a pure state via its Schmidt coefficients, see footnote 3.

and relation (22), we have

$$\sum_{n=1}^{d_2^2-1}\eta_n \leqslant \frac{d_1d_2-1}{d_1d_2} - \frac{d_1-1}{d_1d_2}\|r_1\|^2_{\mathbb{R}^{d_1^2-1}}. \tag{73}$$

We further note that since $\sum_{n=1}^{d_2^2-1}\eta_n = \sum_{n=1}^{d_2-1}\eta_n + \sum_{n=d_2}^{d_2^2-1}\eta_n$ and $\sum_{n=d_2}^{d_2^2-1}\eta_n \leqslant d_2\sum_{n=1}^{d_2-1}\eta_n$, relation (73) implies

$$\sum_{n=d_2}^{d_2^2-1}\eta_n \leqslant \frac{1}{d_2+1}\left\{\frac{d_1d_2-1}{d_1} - \frac{d_1-1}{d_1}\|r_1\|^2_{\mathbb{R}^{d_1^2-1}}\right\}$$
$$= \frac{d_1d_2-1}{d_1(d_2+1)} - \frac{1}{d_2+1}\cdot\frac{d_1-1}{d_1}\|r_1\|^2. \tag{74}$$

By using in (74) equality (20), we derive

$$\sum_{n=d_2}^{d_2^2-1}\eta_n \leqslant \frac{d_1d_2-1}{d_1(d_2+1)} - \frac{1}{d_2+1}\left(\frac{1}{d_2} - \frac{1}{d_1} + \frac{d_2-1}{d_2}\|r_2\|^2\right)$$
$$= \frac{d_2-1}{d_2}\left[1 - \frac{\|r_2\|^2}{d_2+1}\right]. \tag{75}$$

The latter also implies the upper bound (71) and proves the statement. ■

Furthermore, based on the exact relation (46) we find the following general upper and lower bounds on the geometric quantum discord of a two-qudit state.

Theorem 3. For a two-qudit state ρ on $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}$, $d_1, d_2 \geqslant 2$, the geometric quantum discord admits the following bounds:

$$\frac{1}{4}\mathrm{tr}[T_\rho^\dagger T_\rho] - \frac{1}{4}\sum_{n=1}^{d_2-1}\lambda_n \leqslant \mathcal{D}_g(\rho)$$
$$\leqslant \min\left\{\frac{1}{4}\mathrm{tr}[T_\rho^\dagger T_\rho];\ \frac{1}{4}\mathrm{tr}[T_\rho^\dagger T_\rho] + \frac{d_2-1}{d_2d_1}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}} - \frac{1}{4}\sum_{n=1}^{d_2-1}\lambda_n\right\}, \tag{76}$$

where $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \lambda_{d^2-1} \geqslant 0$ are eigenvalues of the positive Hermitian operator $T_\rho^\dagger T_\rho$ on $\mathbb{R}^{d_2^2-1}$.

Proof. For the evaluation of the last term in (43), we note that $\max_x\{f_1(x)+f_2(x)\} \leqslant \max_x f_1(x) + \max_x f_2(x)$ and, if $f_j(x) \geqslant 0$, $j = 1, 2$, then $\max_x\{f_1(x)+f_2(x)\} \geqslant \max_x f_j(x)$, $j = 1, 2$. These relations and Propositions 2 and 4 imply

$$\max_{\Omega_{\Upsilon_{d_2}}}\mathrm{tr}\left[\left(\frac{d_2-1}{d_1d_2}|r_2\rangle\langle r_2| + \frac{1}{4}T_\rho^\dagger T_\rho\right)\Pi_{\Omega_{\Upsilon_{d_2}}}\right]$$
$$\leqslant \max_{\Omega_{\Upsilon_{d_2}}}\mathrm{tr}\left[\frac{d_2-1}{d_1d_2}|r_2\rangle\langle r_2|\Pi_{\Omega_{\Upsilon_{d_2}}}\right] + \max_{\Omega_{\Upsilon_{d_2}}}\mathrm{tr}\left[\frac{1}{4}T_\rho^\dagger T_\rho\Pi_{\Omega_{\Upsilon_{d_2}}}\right]$$
$$= \frac{d_2-1}{d_1d_2}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}} + \frac{1}{4}\sum_{n=1}^{d_2-1}\lambda_n, \tag{77}$$

as well as

$$\max_{\Omega_{\Upsilon_{d_2}}}\mathrm{tr}\left[\left(\frac{d_2-1}{d_1d_2}|r_2\rangle\langle r_2| + \frac{1}{4}T_\rho^\dagger T_\rho\right)\Pi_{\Omega_{\Upsilon_{d_2}}}\right]$$
$$\geqslant \max_{\Omega_{\Upsilon_{d_2}}}\mathrm{tr}\left[\left(\frac{d_2-1}{d_1d_2}|r_2\rangle\langle r_2|\right)\Pi_{\Omega_{\Upsilon_{d_2}}}\right] = \frac{d_2-1}{d_1d_2}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}} \tag{78}$$

and

$$\max_{\Omega_{\Upsilon_{d_2}}}\mathrm{tr}\left[\left(\frac{d_2-1}{d_1d_2}|r_2\rangle\langle r_2| + \frac{1}{4}T_\rho^\dagger T_\rho\right)\Pi_{\Omega_{\Upsilon_{d_2}}}\right]$$
$$\geqslant \max_{\Omega_{\Upsilon_{d_2}}}\mathrm{tr}\left[\frac{1}{4}T_\rho^\dagger T_\rho\Pi_{\Omega_{\Upsilon_{d_2}}}\right] = \frac{1}{4}\sum_{n=1}^{d_2-1}\lambda_n. \tag{79}$$

Relations (77), (78), and (79) prove the statement. ■

From relation (22) and the upper bound in (76) it follows that, for a two qudit state ρ on $\mathcal{H}_{d_1}\otimes\mathcal{H}_{d_2}$, $d_1, d_2 \geqslant 2$,

$$\mathcal{D}_g(\rho) \leqslant \min\{J_1, J_2\}, \tag{80}$$

where

$$J_1 = \frac{d_1d_2-1}{d_2d_1} - \frac{d_1-1}{d_2d_1}\|r_1\|^2_{\mathbb{R}^{d_1^2-1}} - \frac{d_2-1}{d_2d_1}\|r_2\|^2_{\mathbb{R}^{d_2^2-1}} \tag{81}$$

and

$$J_2 = \frac{d_1d_2-1}{d_2d_1} - \frac{d_1-1}{d_2d_1}\|r_1\|^2_{\mathbb{R}^{d_1^2-1}} - \frac{1}{4}\sum_{n=1}^{d_2-1}\lambda_n. \tag{82}$$

Theupper bounds (70) and (71) in Theorem 2 and the upper bounds (76) and (80)–(82) considerably improve the upper bound in Proposition 3.1 of [19] having in our notations the form $\frac{d_1d_2-1}{d_2d_1}$.

Consider also the upper bound on the geometric quantum discord in a general separable case.

Proposition 3. For every separable two-qudit state

$$\rho_{\text{sep}} = \sum_k \beta_k\rho_1^{(k)}\otimes\rho_2^{(k)}, \quad \beta_k \geqslant 0, \quad \sum_k\beta_k = 1, \tag{83}$$

on $\mathcal{H}_d\otimes\mathcal{H}_d$, $d \geqslant 2$,

$$\mathcal{D}_g(\rho_{\text{sep}}) \leqslant \left(\frac{d-1}{d}\right)^2. \tag{84}$$

Proof. In view of expression (27) for the correlation matrix $T_{\rho_{\text{sep}}}$ of separable state ρ_{sep}, we have in case $d_1 = d_2$

$$\frac{1}{4}\mathrm{tr}[T_{\rho_{\text{sep}}}^\dagger T_{\rho_{\text{sep}}}] = \left(\frac{d-1}{d}\right)^2\sum_{k,k_1}\beta_k\beta_{k_1}\left(r_1^{(k)}\cdot r_1^{(k_1)}\right)\left(r_2^{(k)}\cdot r_2^{(k_1)}\right)$$
$$\leqslant \left(\frac{d-1}{d}\right)^2, \tag{85}$$

where $r_j^{(k)}$ are the Bloch vectors of states $\rho_j^{(k)}$, $j = 1, 2$, given by (5) with norms $||r_1^{(k)}||, ||r_2^{(k)}|| \leqslant 1$. ■

From the upper bound (84) it follows that, for any separable two-qubit state, the geometric quantum discord cannot exceed 1/4.

If a separable state is pure, then $||r_1|| = ||r_2|| = 1$ and by (27) the positive Hermitian operator (47) takes the form

$$G\big(\rho_{\text{sep}}^{(\text{pure})}\big) = \frac{d-1}{d^2}|r_2\rangle\langle r_2| + \left(\frac{d-1}{d}\right)^2 \|r_1\|^2 |r_2\rangle\langle r_2| = \left[\frac{d-1}{d^2} + \left(\frac{d-1}{d}\right)^2\right]|r_2\rangle\langle r_2| = \frac{d-1}{d}|r_2\rangle\langle r_2| \tag{86}$$

and has only one nonzero eigenvalue

$$\eta_1 = \frac{d-1}{d} = \text{tr}\big[G\big(\rho_{\text{sep}}^{(\text{pure})}\big)\big] \tag{87}$$

with multiplicity one. Therefore, for a pure separable state, relation (46) gives $\mathcal{D}_g(\rho_{\text{sep}}^{(\text{pure})}) = 0$—as it should be since a pure separable state is quantum classical. This is also consistent with (59) since for a pure separable state the concurrence is equal to zero.

V. CONCLUSION

In the present article, for an arbitrary two-qudit state with any dimensions at two sites, we find (Theorem 1) in the explicit analytical form the exact value of its geometric quantum discord. This rigorously proved general result indicates that the lower bound on the geometric quantum discord found in [15] constitutes its exact value for each two-qudit state and includes only as particular cases the exact results for a general two-qubit state [11], a general qubit-qudit state [15], and some special families of two-qudit states [15,17].

Based on this general result (46) of Theorem 1, we (a) show (Corollary 1) that, for every pure two-qudit state, the exact value of the geometric quantum discord is equal to one-half of its squared concurrence, (b) find (Theorem 2) general upper bounds (70) and (71) on the geometric quantum discord of an arbitrary two-qudit quantum state of any dimensions which are consistent with the exact value in Corollary 1 for the geometric quantum discord of a maximally entangled pure two-qudit state, (c) derive (Theorem 3) for an arbitrary two-qudit state the general upper and lower bounds on the geometric quantum discord expressed via the eigenvalues of its correlation matrix (these upper bounds are tighter than the ones in [19]), and (d) specify (Proposition 3) the upper bound on the geometric quantum discord of an arbitrary separable two-qudit state of any dimension.

The general results derived in the present article considerably extend the range of known results on properties of the geometric quantum discord of a two-qudit state, pure or mixed, of an arbitrary dimension.

As shown in [46,47], there exist bipartite quantum states which, under evolution via some quantum channels, exhibit a particular type of decoherence with the following dynamics of correlations: until some critical value of time only classical correlations are being destroyed while a decrease of quantum correlations starts only after this critical time and this decrease is quantified via the quantum discord. This phenomenon, referred to as the sudden transition of quantum correlations, occurs even in situations where entanglement is monotonically decreasing since the initial time.

Even if under decoherence scenarios the geometric quantum discord could be more fragile than the quantum discord, as it is exemplified for diverse channels in [48], this measure of quantum correlations is a useful concept to analyze quantum correlations dynamics and by using this measure phenomena like the sudden transition have been observed for some three- and six-qubit GHZ states [48]. Similar studies for other N-qubit states were explored recently in [24] and also in [23].

The latter investigations [23,24,48] indicate that our explicit exact analytical expression (46) for the geometric quantum discord could be a fundamental tool to study under diverse decoherence the time evolution of quantum correlations in a general two-qudit system, where, to our knowledge, this measure has not been explored. A possible other application of the geometric quantum discord is to quantify usefulness of a given state for teleportation tasks as long as it interacts with the environment [49].

We also expect that our results will be of relevance in the growing field of relativistic quantum information. We can see the first steps on this direction by recent applications [31,32] of geometric quantum discord for quantifying quantum correlations in quantum gravity contexts.

With these investigations [23,24,48,49] in mind, we believe that our results on the geometric quantum discord for an arbitrary two-qudit state are important not only from the general theoretical point of view but also for the use of this measure of quantum correlations in many practical tasks involving two-qudit systems.

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APPENDIX

The proof of Lemma 1. In view of relations (37), we have

$$\begin{aligned}
\Pi^2_{\Omega_{\Upsilon_d}} &= \left(\frac{d-1}{d}\right)^2 \sum_{k,l\in\{1,\dots,d\}} |y_k\rangle\langle y_k|y_l\rangle\langle y_l| \\
&= \left(\frac{d-1}{d}\right)^2 \sum_{k=1,\dots,d} |y_k\rangle\langle y_k| - \frac{d-1}{d^2} \sum_{k\neq l\in\{1,\dots,d\}} |y_k\rangle\langle y_l| \\
&= \left(\frac{d-1}{d}\right)^2 \sum_{k=1,\dots,d} |y_k\rangle\langle y_k| \\
&\quad - \frac{d-1}{d^2} \sum_{k,l\in\{1,\dots,d\}} |y_k\rangle\langle y_l| + \frac{d-1}{d^2} \sum_{k=1,\dots,d} |y_k\rangle\langle y_k| \\
&= \frac{d-1}{d} \sum_{k=1,\dots,d} |y_k\rangle\langle y_k| = \Pi_{\Omega_{\Upsilon_d}}.
\end{aligned} \tag{A1}$$

Since

$$\text{tr}\big[\Pi_{\Omega_{\Upsilon_d}}\big] = d-1, \tag{A2}$$

the rank of every projection $\Pi_{\Omega_{\Upsilon_d}}$ is equal to $(d-1)$.

Note that an orthogonal projection $\Pi_{\Omega_{\Upsilon_d}}$ has eigenvalue 1 of multiplicity $(d-1)$ and eigenvalue 0 of multiplicity $d(d-1)$. Relations (A1) and (A2) prove Lemma 1. ■

The proof of Theorem 1 implies the following general statement, which we use for finding the bounds in Theorem 3.

Proposition 4. For an arbitrary positive Hermitian operator A on $\mathbb{R}^{d^2-1}$ and the orthogonal projections

$$\Pi_{\Omega_y} = \frac{d-1}{d}\sum_{k=1}^{d} |y_k\rangle\langle y_k|, \tag{A3}$$

on $\mathbb{R}^{d^2-1}$ of rank $d-1$, which are specified in Lemma 1, the maximum

$$\max_{\Omega_y} \operatorname{tr}[A\Pi_{\Omega_y}] = \zeta_1 + \cdots + \zeta_{d-1}, \tag{A4}$$

where $\zeta_1 \geqslant \zeta_2 \geqslant \cdots \geqslant \zeta_{d^2-1} \geqslant 0$ are the eigenvalues of A listed in decreasing order with the corresponding algebraic multiplicities.

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