

# Hilbert-Schmidt measure of pairwise quantum discord for three-qubit $X$ states

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## Abstract

The Hilbert-Schmidt distance between a mixed three-qubit state and its closest state is used to quantify the amount of pairwise quantum correlations in a tripartite system. Analytical expressions of geometric quantum discord are derived. A particular attention is devoted to two special classes of three-qubit  $X$  states. They include three-qubit states of W, GHZ and Bell type. We also discuss the monogamy property of geometric quantum discord in some mixed three-qubit systems.

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# 1 Introduction

Quantum correlations in multipartite systems have been intensively investigated during the last two decades in the context of quantum information science. This is mainly motivated by the fact that quantum correlations constitute a key resource for many quantum information processing tasks (see for instance [1, 2, 3, 4]). Also, the understanding of the basic features of quantum correlations is essential to provide a comprehensive way to distinguish the frontier between quantum and classical physics. Nowadays, quantum correlations have become an important tool in studying several aspects in many-body systems such as quantum phase transition in strongly correlated systems. A rigorous quantitative and qualitative way to decide about the existence of quantum correlation, between the compounds of a composite system, remains an open problem. Various measures to quantify the degree of quantumness in multipartite quantum systems have been discussed in the literature from different perspectives and for several purposes (for a recent review see [5]). Among these several quantifiers of non-classicality, concurrence and entanglement of formation [6, 7] have attracted considerable attention. But, recently it was realized that entanglement of formation does not reveal all non classical aspects of quantum correlations. In this sense, quantum discord was introduced to capture the essential of quantum correlations in composite quantum systems. This measure, which goes beyond entanglement of formation, is defined as the difference between the total amount of nonclassical mutual information and classical correlation present in a bipartite system [8, 9]. The explicit expression of quantum discord requires an optimization procedure that is in general a challenging task. To overcome this problem, a geometric variant of quantum discord was proposed in [10]. Geometric quantum discord was explicitly evaluated between qubit-qubit as well as qubit-qudit systems (see [11] and references therein). In the literature, a particular attention was devoted to quantum correlations in the so-called two-qubit  $X$  states [12-21, 23-27]. In the computational basis, these states have non-zero entries only along the diagonal and anti-diagonal and look like the alphabet  $X$ . Their algebraic structures [28] simplify many analytical calculation in deriving entanglement of formation [29] and quantum discord [14, 25, 30]. Interestingly, algebraic aspects of multi-qubit states have been generalized to describe  $X$  states of quantum systems encompassing more than two qubits [31]. The generalized  $X$  states cover a large class of multi-qubit states including W [32, 33], GHZ [34] and Dicke states [35].

The study of genuine correlations in multipartite quantum systems is complex from conceptual as well as computational point of view. Various approaches, inspired by the results obtained of bipartite systems, were discussed in the literature to tackle this issue. In this paper, we extend the geometric measure of quantum discord for two qubits, to tripartite systems comprising three qubits. The focus will be maintained strictly on two special families of three-qubit  $X$  states for which the explicit expressions of quantum discord are explicitly derived using the Hilbert-Schmidt norm. In other hand, another important question in systems, comprising more than two parts, concerns the distribution of quantum correlations among the subsystems and it is constrained by the the so-called monogamy

relation. In fact, denoting by  $Q$  a bipartite measure of quantum correlations in a tripartite system  $1-2-3$ , the sum of quantum correlations  $Q_{1|2}$  (the shared correlation between 1 and 2) and  $Q_{1|3}$  (the shared correlation between 1 and 3) is always less or equal to the correlation  $Q_{1|23}$  shared between 1 and the composite subsystem 23. The concept of monogamy was introduced by Coffman, Kundo and Wootters in 2001 [36] in investigating the distribution of entanglement in three qubit systems. The monogamy property was analyzed for other measures of quantum correlations to understand the distribution of correlations in multipartite systems and to establish the conditions limiting the shareability of quantum correlations. The entanglement of formation [37, 38], quantum discord [39, 40, 41, 42, 43] and its geometrized variant [44, 45, 46] do not follow in general the monogamy property, contrarily to squared concurrence [36].

This paper is organized as follows. In section 2, we introduce two families of three-qubit  $X$  states. The first one is given by three-qubit states where a subsystem comprising two qubits possesses parity invariance. The second class corresponds to the situation where the three qubits are all invariant under parity symmetry. In section 3, we derive the geometric measure of quantum discord. We also give the explicit forms of classical tripartite states presenting zero discord. To investigate the monogamy property in three-qubit  $X$  states, we give the general expression of geometric quantum discord in reduced states containing two qubits after tracing-out the third qubit in the global quantum state. The explicit expressions of resulting pairwise quantum discord are derived in section 4. To illustrate our calculations, we consider some special instances of three qubit systems for which geometric quantum correlations are given. In addition, we discuss the distribution of geometric quantum discord to decide about the monogamy property. Illustrations for some specific three-qubit mixed states are given. Concluding remarks close this paper.

## 2 Three-qubit $X$ states

$X$  states of two qubits have already found applications in many studies of entanglement and discord [12-27]. As mentioned in the introduction, the interest in generalized  $X$  states is motivated by the fact that they cover many different states of interest in quantum information such as W and GHZ and Dicke states. The generalized  $X$  states are of paramount importance in investigating quantum correlations for a collection of spin-1/2 particles possessing discrete symmetries like particle exchange symmetry and/or parity invariance. For instance, the reduced density matrices of multipartite Schrödinger cat states, which are invariant under permutation symmetry, are  $X$  structured operators (see for instance the reference [47]). Completely symmetric systems, including Dicke states, are relevant in many experimental situations such as spin squeezing which may have potential applications in atomic interferometers and high atomic clocks (see [48] and references therein). Also, The multi-qubit  $X$  states arise naturally in describing the dynamics tripartite quantum spin states interacting with a large environment [49]. This is of crucial importance in analyzing the decoherence effects induced by

the environment in such systems.

In Fano-Bloch representation, a two qubit state writes as

$$\rho_{12} = \frac{1}{4} \sum_{\alpha, \beta=0}^4 T_{\alpha\beta} \sigma_{\alpha} \otimes \sigma_{\beta} \quad (1)$$

where the Fano-Bloch parameters are given by  $T_{\alpha\beta} = \text{Tr}(\rho_{12} \sigma_{\alpha} \otimes \sigma_{\beta})$  and  $\sigma_{\alpha}$  are the Pauli matrices. The symmetry of two qubit systems is fully characterized by the algebra  $\text{su}(4)$  spanned by the  $4 \times 4$  Pauli matrices (see [28, 29, 30] and references therein). An interesting family of two-qubit states which is relevant in several problems of quantum optics and quantum information is the subset whose density matrices resemble the letter  $X$ . They especially arise in physical systems possessing parity symmetry such as Werner, Bell-diagonal and Dicke states. The  $X$  states are parameterized by seven real parameters (three real parameters along the diagonal and two complex parameters at off-diagonal positions). The underlying symmetry is characterized by the sub-algebra  $\text{su}(2) \times \text{u}(1) \times \text{su}(2) \subset \text{su}(4)$  spanned by seven linearly independent generators. Specifically,  $X$  states can be written as

$$\rho_{12} = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix}. \quad (2)$$

in the computational basis for two qubits ( $|00\rangle, |01\rangle, |10\rangle, |11\rangle$ ) or equivalently ( $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$ ) in two spin basis. Clearly, the states of the form (2) commute with the operator  $\sigma_3 \otimes \sigma_3$  reflecting the invariance under parity transformation. The tools developed for two qubit systems are of paramount importance for three or more qubits. The  $X$  states for multi-qubit systems and their underlying symmetries were discussed in [11, 28, 29, 30]. In this paper we shall mainly focus on three-qubits  $X$  states. We consider a tripartite system  $1-2-3$  with each party holding a qubit. The state shared between three parties 1, 2 and 3 is given by the unit trace operator  $\rho_{123}$  acting on the tensor-product Hilbert space  $\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3$  where each single Hilbert space is two-dimensional spanned by the vectors  $|0\rangle$  and  $|1\rangle$ . The three qubit system lives in a  $2^3$ -dimensional Hilbert space. As mentioned in the introduction, two types of  $X$  states are studied in this work. The first type concerns the states commuting with the operator  $\sigma_3 \otimes \sigma_3 \otimes \sigma_0$  and the second class corresponds to density matrices that commute with the operators  $\sigma_3 \otimes \sigma_3 \otimes \sigma_3$ .

## 2.1 Three-qubit $X$ states: first class

The first family of three-qubit states, that we introduce in this section, corresponds to density matrices commuting  $\sigma_3 \otimes \sigma_3 \otimes \sigma_0$ . The states of the subsystem  $1-2$  of the tripartite system  $1-2-3$  are invariant under parity transformation. It is simply verified that, in the usual  $2^3$ -dimensional computational basis, the general form of such states is

$$\rho_{123} = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} & \rho_{15} & 0 & 0 & \rho_{18} \\ 0 & \rho_{22} & \rho_{23} & 0 & 0 & \rho_{26} & \rho_{27} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 & 0 & \rho_{36} & \rho_{37} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} & \rho_{45} & 0 & 0 & \rho_{48} \\ \rho_{51} & 0 & 0 & \rho_{54} & \rho_{55} & 0 & 0 & \rho_{58} \\ 0 & \rho_{62} & \rho_{63} & 0 & 0 & \rho_{66} & \rho_{67} & 0 \\ 0 & \rho_{72} & \rho_{73} & 0 & 0 & \rho_{76} & \rho_{77} & 0 \\ \rho_{81} & 0 & 0 & \rho_{84} & \rho_{85} & 0 & 0 & \rho_{88} \end{pmatrix}. \quad (3)$$

In the Fano-Bloch representation, the three-qubit state (3) takes the following form

$$\rho_{123} = \frac{1}{8} \sum_{\alpha\beta\gamma} \mathcal{R}_{\alpha\beta\gamma} \sigma_{\alpha} \otimes \sigma_{\beta} \otimes \sigma_{\gamma} \quad (4)$$

where  $\alpha, \beta$  and  $\gamma$  take the values  $=0, 1, 2, 3$  and the correlation matrix elements  $\mathcal{R}_{\alpha\beta\gamma}$  are

$$\mathcal{R}_{\alpha\beta\gamma} = \text{Tr}(\rho_{123}(\sigma_{\alpha} \otimes \sigma_{\beta} \otimes \sigma_{\gamma}))$$

with  $\mathcal{R}_{000} = 1$  ( $\text{Tr}(\rho_{123}) = 1$ ). The operators  $\sigma_{\alpha}$  stands for Pauli basis with  $\sigma_0$  is the identity. The parity invariance reduces the number of the non vanishing correlation matrix elements  $\mathcal{R}_{\alpha\beta\gamma}$  in equation (4). Indeed, it is easy to verify that the non vanishing ones are those corresponding to  $(\alpha, \beta, \gamma)$  belonging to the following set of triplets

$$\begin{aligned} &(000), (001), (002), (003), (030), (031), (032), (033) \\ &(110), (111), (112), (113), (120), (121), (122), (123) \\ &(210), (211), (212), (213), (220), (221), (222), (223) \\ &(300), (301), (302), (303), (330), (331), (332), (333). \end{aligned} \quad (5)$$

Accordingly, the state (4) expand as

$$\begin{aligned} \rho_{123} = \frac{1}{8} &\left[ \mathcal{R}_{000} \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \sum_i (\mathcal{R}_{i00} \sigma_i \otimes \sigma_0 \otimes \sigma_0 + \mathcal{R}_{0i0} \sigma_0 \otimes \sigma_i \otimes \sigma_0 + \mathcal{R}_{00i} \sigma_0 \otimes \sigma_0 \otimes \sigma_i) \right. \\ &\left. + \sum_{ij} (\mathcal{R}_{ij0} \sigma_i \otimes \sigma_j \otimes \sigma_0 + \mathcal{R}_{i0j} \sigma_i \otimes \sigma_0 \otimes \sigma_j + \mathcal{R}_{0ij} \sigma_0 \otimes \sigma_i \otimes \sigma_j) + \sum_{ijk} \mathcal{R}_{ijk} \sigma_i \otimes \sigma_j \otimes \sigma_k \right], \end{aligned} \quad (6)$$

in terms of 32 operators which span the subalgebra  $\text{su}(2) \otimes \text{u}(1) \otimes \text{su}(2) \otimes \text{u}(1) \otimes \text{su}(2) \otimes \text{u}(1) \otimes \text{su}(2)$  of the full symmetry algebra  $\text{su}(8)$  characterizing an arbitrary three-qubit system [28, 29, 30]. The explicit relation between the non vanishing Fano-Bloch parameters  $\mathcal{R}_{\alpha\beta\gamma}$  and the matrix elements of  $\rho_{123}$  will be given here after. It is interesting to note that density matrix (3) encompasses four two qubit  $X$  states (four sub-blocks, each one is  $X$  shaped). In fact, the matrix (3) can be written as

$$\rho_{123} = \sum_{i,j=0,1} \rho^{ij} \otimes |i\rangle\langle j| \quad (7)$$

where the vectors  $|i\rangle$  and  $|j\rangle$  are related to the qubit 3. From equation (3), the density matrices  $\rho^{ij}$  appearing in (7) write as

$$\rho^{ij} = \begin{pmatrix} \rho_{1+4i \ 1+4j} & 0 & 0 & \rho_{1+4i \ 4+4j} \\ 0 & \rho_{2+4i \ 2+4j} & \rho_{2+4i \ 3+4j} & 0 \\ 0 & \rho_{3+4i \ 2+4j} & \rho_{3+4i \ 3+4j} & 0 \\ \rho_{4+4i \ 1+4j} & 0 & 0 & \rho_{4+4i \ 4+4j} \end{pmatrix}, \quad (8)$$

in the computational basis spanned by two-qubit product states of 1 and 2  $\{|0\rangle_1 \otimes |0\rangle_2, |0\rangle_1 \otimes |1\rangle_2, |1\rangle_1 \otimes |0\rangle_2, |1\rangle_1 \otimes |1\rangle_2\}$ . The Fano-Bloch representations of the two qubit  $X$  states  $\rho^{ij}$  (8) are

$$\rho^{ij} = \frac{1}{4} \sum_{\alpha\beta} R_{\alpha\beta}^{ij} \sigma_\alpha \otimes \sigma_\beta \quad (9)$$

where  $\alpha, \beta = 0, 1, 2, 3$  and the Fano-Bloch parameters  $R_{\alpha\beta}^{ij}$  defined by

$$R_{\alpha\beta}^{ij} = \text{Tr}(\rho^{ij} \sigma_\alpha \otimes \sigma_\beta),$$

are given by

$$\begin{aligned} R_{00}^{ij} &= 1 \\ R_{30}^{ij} &= \rho_{1+4i \ 1+4j} + \rho_{2+4i \ 2+4j} - \rho_{3+4i \ 3+4j} - \rho_{4+4i \ 4+4j} \\ R_{03}^{ij} &= \rho_{1+4i \ 1+4j} - \rho_{2+4i \ 2+4j} + \rho_{3+4i \ 3+4j} - \rho_{4+4i \ 4+4j} \\ R_{11}^{ij} &= \rho_{1+4i \ 4+4j} + \rho_{4+4i \ 1+4j} + \rho_{2+4i \ 3+4j} + \rho_{3+4i \ 2+4j} \\ R_{12}^{ij} &= i(\rho_{1+4i \ 4+4j} - \rho_{4+4i \ 1+4j} - \rho_{2+4i \ 3+4j} + \rho_{3+4i \ 2+4j}) \\ R_{21}^{ij} &= i(\rho_{1+4i \ 4+4j} - \rho_{4+4i \ 1+4j} + \rho_{2+4i \ 3+4j} - \rho_{3+4i \ 2+4j}) \\ R_{22}^{ij} &= \rho_{2+4i \ 3+4j} + \rho_{3+4i \ 2+4j} - \rho_{1+4i \ 4+4j} - \rho_{4+4i \ 1+4j} \\ R_{33}^{ij} &= \rho_{1+4i \ 1+4j} - \rho_{2+4i \ 2+4j} - \rho_{3+4i \ 3+4j} + \rho_{4+4i \ 4+4j}. \end{aligned} \quad (10)$$

By inserting the Fano-Bloch representations (9) into the expression (7), the tripartite correlations elements  $\mathcal{R}_{\alpha\beta\gamma}$  can be written in terms of the bipartite correlation parameters  $R_{\alpha\beta}^{ij}$ . Indeed, equation (7) can be rewritten as

$$\rho_{123} = \frac{1}{2} \left[ (\rho^{00} + \rho^{11}) \otimes \sigma_0 + (\rho^{00} - \rho^{11}) \otimes \sigma_3 + (\rho^{01} + \rho^{10}) \otimes \sigma_1 + i(\rho^{01} - \rho^{10}) \otimes \sigma_2 \right] \quad (11)$$

and similarly, we rewrite (6) as

$$\rho_{123} = \frac{1}{8} \sum_{\alpha\beta} \left[ \mathcal{R}_{\alpha\beta 0} \sigma_\alpha \otimes \sigma_\beta \otimes \sigma_0 + \mathcal{R}_{\alpha\beta 1} \sigma_\alpha \otimes \sigma_\beta \otimes \sigma_1 + \mathcal{R}_{\alpha\beta 2} \sigma_\alpha \otimes \sigma_\beta \otimes \sigma_2 + \mathcal{R}_{\alpha\beta 3} \sigma_\alpha \otimes \sigma_\beta \otimes \sigma_3 \right]. \quad (12)$$

By Replacing the expressions (9) and (10) in (11), and identifying with the equation (12), one gets

$$\mathcal{R}_{\alpha\beta 0} = R_{\alpha\beta}^{++} = R_{\alpha\beta}^{00} + R_{\alpha\beta}^{11}$$

$$\begin{aligned}
\mathcal{R}_{\alpha\beta 3} &= R_{\alpha\beta}^{--} = R_{\alpha\beta}^{00} - R_{\alpha\beta}^{11} \\
\mathcal{R}_{\alpha\beta 1} &= R_{\alpha\beta}^{+-} = R_{\alpha\beta}^{01} + R_{\alpha\beta}^{10} \\
\mathcal{R}_{\alpha\beta 2} &= R_{\alpha\beta}^{-+} = iR_{\alpha\beta}^{01} - iR_{\alpha\beta}^{10}.
\end{aligned} \tag{13}$$

where the pairs  $(\alpha\beta)$  belong to the set  $\{(00), (03), (30), (12), (21), (11), (22), (33)\}$ . The relations (13) specify completely the tripartite correlation tensor  $\mathcal{R}_{\alpha\beta\gamma}$  in terms of the Fano-Bloch parameters  $R_{\alpha\beta}^{ij}$  encoding the correlations in the two qubit subsystem 1 – 2 (9). As we shall discuss, these recursive relations play a central role in deriving the geometric measure of quantum discord.

## 2.2 Three-qubit $X$ states: second class

Now we consider three-qubit states, denoted by  $\sigma_{123}$ , possessing the symmetry invariance under the parity transformation  $\mathbb{Z}_2 \otimes \mathbb{Z}_2 \otimes \mathbb{Z}_2$ . As they commute with the parity operator  $\sigma_3 \otimes \sigma_3 \otimes \sigma_3$ , they write

$$\sigma_{123} = \begin{pmatrix} \sigma_{11} & 0 & 0 & \sigma_{14} & 0 & \sigma_{16} & \sigma_{17} & 0 \\ 0 & \sigma_{22} & \sigma_{23} & 0 & \sigma_{25} & 0 & 0 & \sigma_{28} \\ 0 & \sigma_{32} & \sigma_{33} & 0 & \sigma_{35} & 0 & 0 & \sigma_{38} \\ \sigma_{41} & 0 & 0 & \sigma_{44} & 0 & \sigma_{46} & \sigma_{47} & 0 \\ 0 & \sigma_{52} & \sigma_{53} & 0 & \sigma_{55} & 0 & 0 & \sigma_{58} \\ \sigma_{61} & 0 & 0 & \sigma_{64} & 0 & \sigma_{66} & \sigma_{67} & 0 \\ \sigma_{71} & 0 & 0 & \sigma_{74} & 0 & \sigma_{76} & \sigma_{77} & 0 \\ 0 & \sigma_{82} & \sigma_{83} & 0 & \sigma_{85} & 0 & 0 & \sigma_{88} \end{pmatrix} \tag{14}$$

in the standard computational basis. The density matrix  $\sigma_{123}$  is built of four blocks. The diagonal blocks appear as  $X$  alphabet with non-zero density matrix elements only along the diagonal and anti-diagonal contrarily to the two off diagonal blocks which have vanishing elements along the diagonal and anti-diagonal. This gives another family of extended three-qubit  $X$  state (see [28, 29, 30] where such states were originally termed  $X$  states). The underlying symmetry is  $\text{su}(2) \otimes \text{u}(1) \otimes \text{su}(2) \otimes \text{u}(1) \otimes \text{su}(2) \otimes \text{u}(1) \otimes \text{su}(2)$ . In the Fano-Bloch representation, the matrix density (14) expands as

$$\begin{aligned}
\sigma_{123} &= \frac{1}{8} \left[ \mathcal{T}_{000} \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \sum_i (\mathcal{T}_{i00} \sigma_i \otimes \sigma_0 \otimes \sigma_0 + \mathcal{T}_{0i0} \sigma_0 \otimes \sigma_i \otimes \sigma_0 + \mathcal{T}_{00i} \sigma_0 \otimes \sigma_0 \otimes \sigma_i) \right. \\
&\quad \left. + \sum_{ij} (\mathcal{T}_{ij0} \sigma_i \otimes \sigma_j \otimes \sigma_0 + \mathcal{T}_{i0j} \sigma_i \otimes \sigma_0 \otimes \sigma_j + \mathcal{T}_{0ij} \sigma_0 \otimes \sigma_i \otimes \sigma_j) + \sum_{ijk} \mathcal{T}_{ijk} \sigma_i \otimes \sigma_j \otimes \sigma_k \right] \tag{15}
\end{aligned}$$

where the the matrix correlation elements are

$$\mathcal{T}_{\alpha\beta\gamma} = \text{Tr}(\sigma_{123}(\sigma_\alpha \otimes \sigma_\beta \otimes \sigma_\gamma))$$

with  $\mathcal{T}_{000} = 1$  ( $\text{Tr}(\sigma_{123}) = 1$ ). The non vanishing correlation elements  $\mathcal{T}_{\alpha\beta\gamma}$  occurring in (15) are those with a triplet  $(\alpha\beta\gamma)$  in the following list

$$(000), (003), (011), (012), (021), (022), (030), (033)$$

$$\begin{aligned}
& (101), (102), (110), (113), (120), (123), (131), (132) \\
& (201), (202), (210), (213), (220), (223), (231), (232) \\
& (300), (303), (311), (312), (321), (322), (330), (333).
\end{aligned} \tag{16}$$

Analogously to the previous class of three-qubit states, we write the density matrix (14) as

$$\sigma_{123} = \sum_{i,j=0,1} \sigma^{ij} \otimes |i\rangle\langle j| \tag{17}$$

where  $|i\rangle$  and  $|j\rangle$  are eigenvectors associated with the third qubit. In equation (17), the matrices  $\sigma^{ii}$  (with  $i = 0, 1$ ) write, in the computational basis spanned by two-qubit product states of the subsystems 1 and 2  $\{|0\rangle_1 \otimes |0\rangle_2, |0\rangle_1 \otimes |1\rangle_2, |1\rangle_1 \otimes |0\rangle_2, |1\rangle_1 \otimes |1\rangle_2\}$ , as

$$\sigma^{ii} = \begin{pmatrix} \sigma_{1+4i \ 1+4i} & 0 & 0 & \sigma_{1+4i \ 4+4i} \\ 0 & \sigma_{2+4i \ 2+4i} & \sigma_{2+4i \ 3+4i} & 0 \\ 0 & \sigma_{3+4i \ 2+4i} & \sigma_{3+4i \ 3+4i} & 0 \\ \sigma_{4+4i \ 1+4i} & 0 & 0 & \sigma_{4+4i \ 4+4i} \end{pmatrix}. \tag{18}$$

For  $(i = 0, j = 1)$  and  $(i = 1, j = 0)$ , we have

$$\sigma^{ij} = \begin{pmatrix} 0 & \sigma_{1+4i \ 2+4j} & \sigma_{1+4i \ 3+4j} & 0 \\ \sigma_{2+4i \ 1+4j} & 0 & 0 & \sigma_{2+4i \ 4+4j} \\ \sigma_{3+4i \ 1+4j} & 0 & 0 & \sigma_{3+4i \ 4+4j} \\ 0 & \sigma_{4+4i \ 2+4j} & \sigma_{4+4i \ 3+4j} & 0 \end{pmatrix}. \tag{19}$$

The Fano-Bloch representations of the matrices  $\sigma^{ii}$  are

$$\sigma^{ii} = \frac{1}{4} \sum_{\alpha\beta} T_{\alpha\beta}^{ii} \sigma_{\alpha} \otimes \sigma_{\beta} \tag{20}$$

where  $\alpha, \beta = 0, 1, 2, 3$  and the vanishing correlation parameters  $T_{\alpha\beta}^{ij}$  are given by

$$\begin{aligned}
T_{00}^{ii} &= 1 \\
T_{30}^{ii} &= \sigma_{1+4i \ 1+4i} + \sigma_{2+4i \ 2+4i} - \sigma_{3+4i \ 3+4i} - \sigma_{4+4i \ 4+4i} \\
T_{03}^{ii} &= \sigma_{1+4i \ 1+4i} - \sigma_{2+4i \ 2+4i} + \sigma_{3+4i \ 3+4i} - \sigma_{4+4i \ 4+4i} \\
T_{11}^{ii} &= \sigma_{1+4i \ 4+4i} + \sigma_{4+4i \ 1+4i} + \sigma_{2+4i \ 3+4i} + \sigma_{3+4i \ 2+4i} \\
T_{12}^{ii} &= i(\sigma_{1+4i \ 4+4i} - \sigma_{4+4i \ 1+4i} - \sigma_{2+4i \ 3+4i} + \sigma_{3+4i \ 2+4i}) \\
T_{21}^{ii} &= i(\sigma_{1+4i \ 4+4i} - \sigma_{4+4i \ 1+4i} + \sigma_{2+4i \ 3+4i} - \sigma_{3+4i \ 2+4i}) \\
T_{22}^{ii} &= \sigma_{2+4i \ 3+4i} + \sigma_{3+4i \ 2+4i} - \sigma_{1+4i \ 4+4i} - \sigma_{4+4i \ 1+4i} \\
T_{33}^{ii} &= \sigma_{1+4i \ 1+4i} - \sigma_{2+4i \ 2+4i} - \sigma_{3+4i \ 3+4i} + \sigma_{4+4i \ 4+4i}.
\end{aligned} \tag{21}$$



Similarly, for the two-qubit matrices  $\sigma^{ij}$  (19), the corresponding Fano-Bloch representations are

$$\sigma^{ij} = \frac{1}{4} \sum_{\alpha\beta} T_{\alpha\beta}^{ij} \sigma_{\alpha} \otimes \sigma_{\beta} \quad i \neq j \quad (22)$$

where the non zero matrix elements  $T_{\alpha\beta}^{ij}$  are given by

$$\begin{aligned} T_{01}^{ij} &= \sigma_{2+4i \ 1+4j} + \sigma_{1+4i \ 2+4j} + \sigma_{4+4i \ 3+4j} + \sigma_{3+4i \ 4+4j} \\ T_{02}^{ij} &= i(-\sigma_{2+4i \ 1+4j} + \sigma_{1+4i \ 2+4j} - \sigma_{4+4i \ 3+4j} + \sigma_{3+4i \ 4+4j}) \\ T_{10}^{ij} &= \sigma_{1+4i \ 3+4j} + \sigma_{3+4i \ 1+4j} + \sigma_{2+4i \ 4+4j} + \sigma_{4+4i \ 2+4j} \\ T_{13}^{ij} &= \sigma_{1+4i \ 3+4j} + \sigma_{3+4i \ 1+4j} - \sigma_{2+4i \ 4+4j} - \sigma_{4+4i \ 2+4j} \\ T_{20}^{ij} &= i(\sigma_{1+4i \ 3+4j} - \sigma_{3+4i \ 1+4j} + \sigma_{2+4i \ 4+4j} - \sigma_{4+4i \ 2+4j}) \\ T_{23}^{ij} &= i(\sigma_{1+4i \ 3+4j} - \sigma_{3+4i \ 1+4j} - \sigma_{2+4i \ 4+4j} + \sigma_{4+4i \ 2+4j}) \\ T_{31}^{ij} &= \sigma_{1+4i \ 2+4j} + \sigma_{2+4i \ 1+4j} - \sigma_{3+4i \ 4+4j} - \sigma_{4+4i \ 3+4j} \\ T_{32}^{ij} &= i(\sigma_{1+4i \ 2+4j} - \sigma_{2+4i \ 1+4j} - \sigma_{3+4i \ 4+4j} + \sigma_{4+4i \ 3+4j}). \end{aligned} \quad (23)$$

Using (17), one obtains

$$\sigma_{123} = \frac{1}{2} \left[ (\sigma^{00} + \sigma^{11}) \otimes \sigma_0 + (\sigma^{00} - \sigma^{11}) \otimes \sigma_3 + (\sigma^{01} + \sigma^{10}) \otimes \sigma_1 + i(\sigma^{01} - \sigma^{10}) \otimes \sigma_2 \right]. \quad (24)$$

The three-qubit state (15) rewrites also as

$$\sigma_{123} = \frac{1}{8} \sum_{\alpha\beta} \left[ \mathcal{T}_{\alpha\beta 0} \sigma_{\alpha} \otimes \sigma_{\beta} \otimes \sigma_0 + \mathcal{T}_{\alpha\beta 1} \sigma_{\alpha} \otimes \sigma_{\beta} \otimes \sigma_1 + \mathcal{T}_{\alpha\beta 2} \sigma_{\alpha} \otimes \sigma_{\beta} \otimes \sigma_2 + \mathcal{T}_{\alpha\beta 3} \sigma_{\alpha} \otimes \sigma_{\beta} \otimes \sigma_3 \right] \quad (25)$$

Inserting (20) and (22) in the equation (24), one verifies the following relations

$$\begin{aligned} \mathcal{T}_{\alpha\beta 0} &= T_{\alpha\beta}^{++} = T_{\alpha\beta}^{00} + T_{\alpha\beta}^{11} \\ \mathcal{T}_{\alpha\beta 3} &= T_{\alpha\beta}^{--} = T_{\alpha\beta}^{00} - T_{\alpha\beta}^{11} \end{aligned} \quad (26)$$

where  $(\alpha\beta)$  belongs to the set  $\{(00), (03), (30), (12), (21), (11), (22), (33)\}$  and

$$\begin{aligned} \mathcal{T}_{\alpha\beta 1} &= T_{\alpha\beta}^{+-} = T_{\alpha\beta}^{01} + T_{\alpha\beta}^{10} \\ \mathcal{T}_{\alpha\beta 2} &= T_{\alpha\beta}^{-+} = iT_{\alpha\beta}^{01} - iT_{\alpha\beta}^{10} \end{aligned} \quad (27)$$

where  $(\alpha\beta)$  are in the set  $\{(01), (02), (10), (20), (13), (23), (31), (32)\}$ , so that the total number of non vanishing correlation matrix  $\mathcal{T}_{\alpha\beta\gamma}$  elements is 32 to be compared with (16). The relations (26) and (27) reflect that the tensor element  $\mathcal{T}_{\alpha\beta\gamma}$  can be explicitly expressed in terms of two-qubit correlations factors.

### 3 Geometric measure of quantum discord

A bipartite quantum system exhibits quantum correlation if its two subsystems contain more information than taken separately. This concept is captured by the mutual information  $I(A : B) = H(A) + H(B) - H(A, B)$  where  $A$  and  $B$  are random variables. In classical information theory  $H(\cdot)$  stands for the Shannon entropy  $H(p) = -\sum_i p_i \log p_i$  where  $p = (p_1, p_2, \dots)$  is the probability distribution. For a quantum density matrix  $\rho$ ,  $H(\cdot)$  denotes the von Neumann entropy  $H(\rho) = -\text{Tr} \rho \log \rho$ . In the classical case, an equivalent expression for the mutual information is given by  $I(A : B) = H(A) - H(A|B)$  where  $H(A|B)$  is the Shannon entropy of  $A$  conditioned on the measurement outcome of  $B$ . In the quantum case, the two expressions are different and the difference defines the so-called quantum discord [8, 9]. The von Neumann entropy-type quantum discord involves complicated optimization procedures [25]. In the literature there are few examples for which closed analytical expressions for quantum discord were obtained (see the review [5]). Alternatively, distance-type quantifiers of quantum discord have been considered. This is essentially motivated by their presumably simple evaluation in comparison with the original quantum discord definition. Several distances are possible (trace distance, Bures distance, ...) with their own advantages and drawbacks. In this paper we shall especially consider the geometric discord variant based on Hilbert-Schmidt norm [10]. Thus, given a tripartite system  $1 - 2 - 3$ , we shall consider the bipartite splitting  $1|23$ . The pairwise quantum correlation between the subsystems (1) and (23) in three-qubit  $X$  states of type (3) or (14) is determined in complete analogy with two qubit  $X$  state. It is defined as the distance from the set of classically correlated states using Hilbert-Schmidt trace. In this respect, the explicit form of states of type (3) or (14) presenting vanishing quantum correlation can be derived by optimizing the Hilbert-Schmidt norm by means of which quantumness is quantified. This issue constitutes the main of this section.

#### 3.1 Closest classical states to two qubit $X$ states

To begin, we shall present the procedure leading to the closest classically correlated state to the two-qubit  $X$  state (2). The Fano-Bloch representation (1) reads

$$\rho_{12} = \frac{1}{4} \left[ \sigma_0 \otimes \sigma_0 + T_{03} \sigma_0 \otimes \sigma_3 + T_{30} \sigma_3 \otimes \sigma_0 + \sum_{kl} T_{kl} \sigma_k \otimes \sigma_l \right] \quad (28)$$

where the correlation matrix elements are obtainable from (10) modulo some obvious substitutions. The geometric measure of quantum discord is defined as the distance the state  $\rho_{12}$  and its closest classical-quantum state presenting zero discord [10]

$$D_g(\rho_{12}) = \min_{\chi_{12}} \|\rho_{12} - \chi_{12}\|^2 \quad (29)$$

where the Hilbert-Schmidt norm is defined by  $\|X\|^2 = \text{Tr}(X^\dagger X)$  and the minimization is taken over the set of all classical states. When the measurement is performed on the qubit 1, the classical states

write

$$\chi_{12} = p_1 |\psi_1\rangle\langle\psi_1| \otimes \rho_1^2 + p_2 |\psi_2\rangle\langle\psi_2| \otimes \rho_2^2 \quad (30)$$

where  $\{|\psi_1\rangle, |\psi_2\rangle\}$  is an orthonormal basis related to the qubit 1,  $p_i$  ( $i = 1, 2$ ) stands for probability distribution and  $\rho_i^2$  ( $i = 1, 2$ ) is the marginal density of the qubit 2. The classically correlated states  $\chi_{12}$  can also be written as

$$\chi_{12} = \frac{1}{4} \left[ \sigma_0 \otimes \sigma_0 + \sum_{i=1}^3 t e_i \sigma_i \otimes \sigma_0 + \sum_{i=1}^3 (s_+)_i \sigma_0 \otimes \sigma_i + \sum_{i,j=1}^3 e_i (s_-)_j \sigma_i \otimes \sigma_j \right] \quad (31)$$

where

$$t = p_1 - p_2, \quad e_i = \langle\psi_1|\sigma_i|\psi_1\rangle, \quad (s_{\pm})_j = \text{Tr}((p_1\rho_1^2 \pm p_2\rho_2^2)\sigma_j).$$

It follows that the distance between the density matrix  $\rho_{12}$  and the classical state  $\chi_{12}$ , as measured by Hilbert-Schmidt norm, is then given by

$$\|\rho_{12} - \chi_{12}\|^2 = \frac{1}{4} \left[ (t^2 - 2te_3T_{30} + T_{30}^2) + \sum_{i=1}^3 (T_{0i} - (s_+)_i)^2 + \sum_{i,j=1}^3 (T_{ij} - e_i(s_-)_j)^2 \right] \quad (32)$$

The minimization of the distance (32), with respect to the parameters  $t$ ,  $(s_+)_i$  and  $(s_-)_i$ , gives

$$\begin{aligned} t &= e_3 T_{30} \\ (s_+)_1 &= 0 \quad (s_+)_2 = 0 \quad (s_+)_3 = T_{03} \\ (s_-)_i &= \sum_{j=1}^3 e_j T_{ji}. \end{aligned} \quad (33)$$

Inserting these solutions in (32), one has

$$\|\rho_{12} - \chi_{12}\|^2 = \frac{1}{4} \left[ \text{Tr} K - \vec{e}^t K \vec{e} \right] \quad (34)$$

where the matrix  $K$  is defined by

$$K = x x^\dagger + T T^\dagger \quad (35)$$

with

$$x^\dagger = (0, 0, T_{30}) \quad T = \begin{pmatrix} T_{11} & T_{12} & 0 \\ T_{21} & T_{22} & 0 \\ 0 & 0 & T_{33} \end{pmatrix}.$$

From equation (34), one see that the minimal value of Hilbert-Schmidt distance (34) is reached for the largest eigenvalue of the matrix  $K$ . We denote by  $\lambda_1$ ,  $\lambda_2$  and  $\lambda_3$  the eigenvalues of the matrix  $K$  (35) corresponding to the  $X$  state (2) or equivalently (28). They are given by

$$\lambda_1 = 4(|\rho_{14}| + |\rho_{23}|)^2, \quad \lambda_2 = 4(|\rho_{14}| - |\rho_{23}|)^2, \quad \lambda_3 = 2[(\rho_{11} - \rho_{33})^2 + (\rho_{22} - \rho_{44})^2]. \quad (36)$$

To get the minimal value of the Hilbert-Schmidt distance (34) and subsequently the amount of geometric quantum discord, one compares  $\lambda_1$ ,  $\lambda_2$  and  $\lambda_3$ . As  $\lambda_1$  is always greater than  $\lambda_2$ , the largest eigenvalue  $\lambda_{\max}$  is  $\lambda_1$  or  $\lambda_3$ . It follows that the geometric discord is given by

$$D_g(\rho_{12}) = \frac{1}{4} \min\{\lambda_1 + \lambda_2, \lambda_2 + \lambda_3\}. \quad (37)$$

To write down the explicit expressions of the closest classical state  $\chi_{12}$  to  $\rho_{12}$ , one has to determine the eigenvector  $\vec{e}_{\max}$  associated with the largest eigenvalue  $\lambda_{\max}$ . In this respect, two cases ( $\lambda_{\max} = \lambda_1$  and  $\lambda_{\max} = \lambda_3$ ) are separately discussed. We begin by density matrices  $\rho_{12}$  (2) whose entries satisfy the condition  $\lambda_{\max} = \lambda_3$ . The associated eigenvector is given by  $\vec{e}_3 = (0, 0, 1)$ . Replacing in the set of constraints (33), one has

$$\chi_{12}^3 = \frac{1}{4} \begin{bmatrix} \sigma_0 \otimes \sigma_0 + T_{30} & \sigma_3 \otimes \sigma_0 + T_{03} & \sigma_0 \otimes \sigma_3 + T_{33} & \sigma_3 \otimes \sigma_3 \end{bmatrix} \quad (38)$$

In the second situation, the eigenvector corresponding to  $\lambda_1$  is given by  $\vec{e}_1 = (\cos \frac{\phi}{2}, -\sin \frac{\phi}{2}, 0)$  where  $e^{i\phi} = \frac{\rho_{14}\rho_{23}}{|\rho_{14}||\rho_{23}|}$ . Reporting the components of  $\vec{e}_1$  in (33), one gets the closest classical state

$$\chi_{12}^1 = \frac{1}{4} \left[ \sigma_0 \otimes \sigma_0 + T_{30} \sigma_3 \otimes \sigma_0 + \sum_{i=1}^2 \sum_{j=1}^2 \tilde{T}_{ij} \sigma_i \otimes \sigma_j \right] \quad (39)$$

where

$$\begin{aligned} \tilde{T}_{11} &= \cos \frac{\phi}{2} (\cos \frac{\phi}{2} T_{11} - \sin \frac{\phi}{2} T_{21}) & \tilde{T}_{12} &= \cos \frac{\phi}{2} (\cos \frac{\phi}{2} T_{12} - \sin \frac{\phi}{2} T_{22}) \\ \tilde{T}_{21} &= -\sin \frac{\phi}{2} (\cos \frac{\phi}{2} T_{11} - \sin \frac{\phi}{2} T_{21}) & \tilde{T}_{22} &= -\sin \frac{\phi}{2} (\cos \frac{\phi}{2} T_{12} - \sin \frac{\phi}{2} T_{22}). \end{aligned}$$

As we already mentioned, the geometric quantifiers of quantum correlations in bipartite systems can be extended to embrace three-qubit  $X$  states of type (3) or (14).

### 3.2 Closest classical states to three-qubits $X$ states

Along similar lines of reasoning, we determine first the closest classical states to generalized  $X$  states of the form  $\rho_{123}$  (3) and  $\sigma_{123}$  (14). The algebraic structures of both three-qubit density matrices offer many simplification in quantifying geometric quantum discord. To deal with the states  $\rho_{123}$  (3) and  $\sigma_{123}$  (14) in a common framework, it is interesting to note that  $\rho_{123}$  as well as  $\sigma_{123}$  have a similar Fano-Bloch representation. That is

$$\varrho_{123} = \frac{1}{8} \left[ T_{000} \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + T_{300} \sigma_3 \otimes \sigma_0 \otimes \sigma_0 + \sum_{(\beta, \gamma) \neq (0,0)} T_{0\beta\gamma} \sigma_0 \otimes \sigma_\beta \otimes \sigma_\gamma + \sum_i \sum_{(\beta, \gamma) \neq (0,0)} T_{i\beta\gamma} \sigma_i \otimes \sigma_\beta \otimes \sigma_\gamma \right] \quad (40)$$

where the notation  $T_{\alpha\beta\gamma}$  stands for the correlations coefficients  $\mathcal{R}_{\alpha\beta\gamma}$  (resp.  $\mathcal{T}_{\alpha\beta\gamma}$ ) of the states  $\varrho_{123}$  of type  $\rho_{123}$  (3) (resp.  $\sigma_{123}$  (14)). The evaluation of the geometric quantum discord (29) requires a minimization procedure over the set of all classically correlated states, i.e., the states of the form (31).

In a bipartition of type 1|23, a zero discord state is necessarily of the form

$$\chi_{1|23} = p_1 |\psi_1\rangle\langle\psi_1| \otimes \varrho_1^{23} + p_2 |\psi_2\rangle\langle\psi_2| \otimes \varrho_2^{23} \quad (41)$$

where  $\{|\psi_1\rangle, |\psi_2\rangle\}$  is an orthonormal basis related to the qubit 1. The density matrices  $\varrho_i^{23}$  ( $i = 1, 2$ ) corresponding to the subsystem 23 write as

$$\varrho_i^{23} = \frac{1}{4} \left[ \sum_{\alpha, \beta} \text{Tr}(\varrho_i^{23} \sigma_\alpha \otimes \sigma_\beta) \sigma_\alpha \otimes \sigma_\beta \right].$$

The Fano-Bloch form of the tripartite classical state (41) is

$$\begin{aligned} \chi_{1|23} = & \frac{1}{8} \left[ \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \sum_{i=1}^3 t e_i \sigma_i \otimes \sigma_0 \otimes \sigma_0 \right. \\ & \left. + \sum_{(\alpha, \beta) \neq (0,0)} (s_+)_{\alpha, \beta} \sigma_0 \otimes \sigma_\alpha \otimes \sigma_\beta + \sum_{i=1}^3 \sum_{(\alpha, \beta) \neq (0,0)} e_i (s_-)_{\alpha, \beta} \sigma_i \otimes \sigma_\alpha \otimes \sigma_\beta \right] \end{aligned} \quad (42)$$

where

$$t = p_1 - p_2 \quad e_i = \langle \psi_1 | \sigma_i | \psi_1 \rangle \quad (s_\pm)_{\alpha, \beta} = \text{Tr}((p_1 \varrho_1^{23} \pm p_2 \varrho_2^{23}) \sigma_\alpha \otimes \sigma_\beta).$$

The Hilbert-Schmidt distance between the state  $\varrho_{123}$  (40) and a classical state of type (42) gives

$$\|\varrho_{1|23} - \chi_{1|23}\|^2 = \frac{1}{8} \left[ (t^2 - 2te_3 T_{300} + T_{300}^2) + \sum_{(\alpha, \beta) \neq (0,0)} (T_{0\alpha\beta} - (s_+)_{\alpha, \beta})^2 + \sum_{i=1}^3 \sum_{(\alpha, \beta) \neq (0,0)} (T_{i\alpha\beta} - e_i (s_-)_{\alpha, \beta})^2 \right]. \quad (43)$$

Setting zero the partial derivatives of Hilbert-Schmidt distance (43) with respect to the variables  $t$  and  $(s_\pm)_{\alpha, \beta}$ , one has

$$t = e_3 T_{300} \quad (s_+)_{\alpha, \beta} = T_{0\alpha\beta} \quad (s_-)_{\alpha, \beta} = \sum_{i=1}^3 e_i T_{i\alpha\beta}. \quad (44)$$

Reporting the results (44) in (43), one obtains

$$\|\varrho_{1|23} - \chi_{1|23}\|^2 = \frac{1}{8} \left[ T_{300}^2 - e_3^2 T_{300}^2 + \sum_{i=1}^3 \sum_{(\alpha, \beta) \neq (0,0)} T_{i\alpha\beta}^2 - \sum_{i,j=1}^3 \sum_{(\alpha, \beta) \neq (0,0)} e_i e_j T_{i\alpha\beta} T_{j\alpha\beta} \right] \quad (45)$$

to be optimized with respect to the three components of the unit vector  $\vec{e}^t = (e_1, e_2, e_3)$ . The equation (45) can re-expressed as

$$\|\varrho_{1|23} - \chi_{1|23}\|^2 = \frac{1}{8} [\|x\|^2 + \|T\|^2 - \vec{e}^t (x x^t + T T^t) \vec{e}] \quad (46)$$

in terms of the  $3 \times 1$  matrix  $x$  defined by

$$x^t = (0, 0, T_{300}) \quad (47)$$

and the  $3 \times 15$  matrix given by

$$T = (T_{i\alpha\beta}) \quad \text{with} \quad i = 1, 2, 3 \quad (\alpha, \beta) \neq (0, 0). \quad (48)$$

The minimal value of the Hilbert-Schmidt distance (46) is reached when  $\vec{e}$  is the eigenvector associated with the largest eigenvalue  $k_{\max}$  of the matrix defined by

$$K = x x^t + T T^t. \quad (49)$$

It follows that the minimal value given by

$$D_g(\varrho_{1|23}) = \frac{1}{8}(k_1 + k_2 + k_3 - k_{\max}) \quad (50)$$

is the measure quantifying the pairwise quantum discord in the state  $\varrho_{123}$  divided into the subsystems 1 and 23. Note that the sum of the eigenvalues  $k_1$ ,  $k_2$  and  $k_3$  of the matrix  $K$  is exactly the sum of the Hilbert-Schmidt norms of the matrices  $x$  and  $T$  ( $k_1 + k_2 + k_3 = \|x\|^2 + \|T\|^2$ ). For the state  $\rho_{123}$  (3) as well as  $\sigma_{123}$  (14), the matrix  $K$  takes the form

$$K = \begin{pmatrix} K_{11} & K_{12} & 0 \\ K_{21} & K_{22} & 0 \\ 0 & 0 & K_{33} \end{pmatrix}. \quad (51)$$

The geometric measure of quantum discord is determined in terms of the eigenvalues

$$\begin{aligned} k_1 &= \frac{1}{2}(K_{11} + K_{22}) + \frac{1}{2}\sqrt{(K_{11} + K_{22})^2 - 4(K_{11}K_{22} - K_{12}K_{21})} \\ k_2 &= \frac{1}{2}(K_{11} + K_{22}) - \frac{1}{2}\sqrt{(K_{11} + K_{22})^2 - 4(K_{11}K_{22} - K_{12}K_{21})} \\ k_3 &= K_{33}. \end{aligned} \quad (52)$$

Noticing that  $k_1$  is always greater than  $k_2$ , the geometric quantum discord (50) rewrites as

$$D_g(\varrho_{1|23}) = \frac{1}{4}(k_2 + \min(k_1, k_3)). \quad (53)$$

The minimal Hilbert-Schmidt is obtained for the vector  $\vec{e}$  (see equation (46)) associated with the largest eigenvalue of the matrix  $K$  (51). In this sense, to write the explicit form of closest classical states, one distinguishes two situations:  $k_{\max} = k_1$  or  $k_{\max} = k_3$ . For states  $\varrho_{123}$  with entries satisfying the condition  $k_{\max} = k_1$ , it is easy to verify that the maximal eigenvector is given by

$$\vec{e}_1^t = (\cos \theta, -\sin \theta, 0) \quad \text{with} \quad \tan \theta = \frac{K_{11} - k_1}{K_{12}},$$

and subsequently the closest classical states write

$$\chi_{1|23}^{(1)} = \frac{1}{8} \left[ \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \sum_{(\alpha, \beta) \neq (0, 0)} T_{0\alpha\beta} \sigma_0 \otimes \sigma_\alpha \otimes \sigma_\beta + \sum_{(\alpha, \beta) \neq (0, 0)} T_{1\alpha\beta}^{(1)} \sigma_1 \otimes \sigma_\alpha \otimes \sigma_\beta + \sum_{(\alpha, \beta) \neq (0, 0)} T_{2\alpha\beta}^{(1)} \sigma_2 \otimes \sigma_\alpha \otimes \sigma_\beta \right] \quad (54)$$

where

$$T_{1\alpha\beta}^{(1)} = \cos^2 \theta T_{1\alpha\beta} - \cos \theta \sin \theta T_{2\alpha\beta} \quad T_{2\alpha\beta}^{(1)} = \sin^2 \theta T_{2\alpha\beta} - \cos \theta \sin \theta T_{1\alpha\beta}.$$

For states satisfying  $k_{\max} = k_3$ , the maximal eigenvector is

$$\vec{e}_3^t = (0, 0, 1),$$

and it follows that the closest classical state takes the form

$$\chi_{1|23}^{(3)} = \frac{1}{8} \left[ \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + T_{300} \sigma_3 \otimes \sigma_0 \otimes \sigma_0 + \sum_{(\alpha, \beta) \neq (0, 0)} T_{0\alpha\beta} \sigma_0 \otimes \sigma_\alpha \otimes \sigma_\beta + \sum_{(\alpha, \beta) \neq (0, 0)} T_{3\alpha\beta} \sigma_3 \otimes \sigma_\alpha \otimes \sigma_\beta \right]. \quad (55)$$

It is worth noticing that the entries of the matrix  $K$  defined by (49) can be explicitly expressed in terms of the correlations factors and subsequently in terms of the density matrices elements. Obviously, this will provides us with the analytical expressions of quantum discord (53) in terms the matrix elements of states  $\rho_{123}$  and  $\sigma_{123}$ . This issue is discussed in what follows.

### 3.2.1 States of type $\rho_{123}$

For three-qubit states  $\rho_{123}$  (40) belonging to class of states of type (6), we have

$$\rho_{123} = \frac{1}{8} \left[ \mathcal{R}_{000} \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \mathcal{R}_{300} \sigma_3 \otimes \sigma_0 \otimes \sigma_0 + \sum_{(\beta, \gamma) \neq (0,0)} \mathcal{R}_{0\beta\gamma} \sigma_0 \otimes \sigma_\beta \otimes \sigma_\gamma + \sum_i \sum_{(\beta, \gamma) \neq (0,0)} \mathcal{R}_{i\beta\gamma} \sigma_i \otimes \sigma_\beta \otimes \sigma_\gamma \right]. \quad (56)$$

To obtain the matrix  $K$  (51), we replace the correlations coefficients  $T_{\alpha\beta\gamma}$ , in the matrices  $x$  (47) and  $T$  (48), with their counterparts  $\mathcal{R}_{\alpha\beta\gamma}$ . In this way, after straightforward algebra, one shows

$$K_{ij} = \sum_{k=1}^2 \sum_{l=0}^3 \mathcal{R}_{ikl} \mathcal{R}_{jkl} \quad \text{with } i, j = 1, 2 \quad (57)$$

and

$$K_{33} = \sum_{i=0,3} \sum_{j=0}^3 \mathcal{R}_{3ij}^2. \quad (58)$$

Furthermore, using the relations (13), these quantities are expressed as

$$K_{11} = 2[(R_{11}^{00})^2 + (R_{11}^{11})^2] + 2[(R_{12}^{00})^2 + (R_{12}^{11})^2] + 4[R_{11}^{01} R_{11}^{10} + R_{12}^{01} R_{12}^{10}], \quad (59)$$

$$K_{22} = 2[(R_{21}^{00})^2 + (R_{21}^{11})^2] + 2[(R_{22}^{00})^2 + (R_{22}^{11})^2] + 4[R_{21}^{01} R_{21}^{10} + R_{22}^{01} R_{22}^{10}], \quad (60)$$

$$K_{33} = 2[(R_{30}^{00})^2 + (R_{30}^{11})^2] + 2[(R_{33}^{00})^2 + (R_{33}^{11})^2] + 4[R_{30}^{01} R_{30}^{10} + R_{33}^{01} R_{33}^{10}], \quad (61)$$

$$K_{12} = K_{21} = 2[R_{11}^{00} R_{21}^{00} + R_{11}^{11} R_{21}^{11} + R_{12}^{00} R_{22}^{00} + R_{12}^{11} R_{22}^{11}] + 2[R_{11}^{10} R_{21}^{01} + R_{11}^{01} R_{21}^{10} + R_{12}^{10} R_{22}^{01} + R_{12}^{01} R_{22}^{10}], \quad (62)$$

in terms of two qubit correlation elements related to the two qubit correlations matrices  $\rho^{ij}$  given by (10). Subsequently, the entries of the matrix  $K$  (51) are

$$K_{11} = 8 \left( |\rho_{23} + \rho_{41}|^2 + |\rho_{67} + \rho_{85}|^2 + |\rho_{36} + \rho_{18}|^2 + |\rho_{54} + \rho_{72}|^2 \right)$$

$$K_{22} = 8 \left( |\rho_{23} - \rho_{41}|^2 + |\rho_{67} - \rho_{85}|^2 + |\rho_{36} - \rho_{18}|^2 + |\rho_{54} - \rho_{72}|^2 \right)$$

$$K_{12} = K_{21} = -16 \left( |\rho_{23}| |\rho_{14}| \sin(\gamma_{23} + \gamma_{14}) + |\rho_{58}| |\rho_{67}| \sin(\gamma_{58} + \gamma_{67}) + |\rho_{18}| |\rho_{36}| \sin(\gamma_{18} - \gamma_{36}) + |\rho_{27}| |\rho_{45}| \sin(\gamma_{27} - \gamma_{45}) \right)$$

$$K_{33} = 4 \left( (\rho_{11} - \rho_{33})^2 + (\rho_{22} - \rho_{44})^2 + (\rho_{55} - \rho_{77})^2 + (\rho_{66} - \rho_{88})^2 + |(\rho_{15} - \rho_{37}) + (\rho_{26} - \rho_{48})|^2 + |(\rho_{15} - \rho_{37}) - (\rho_{26} - \rho_{48})|^2 \right) \quad (63)$$

where  $\gamma_{ij} = \frac{\rho_{ij}}{|\rho_{ij}|}$  for  $i < j$ . The results (63) give the explicit forms of the matrix elements of  $K$ . Clearly, reporting them in (52), one can get the explicit expression of the geometric quantum discord

(53) in terms of the density matrix elements of  $\rho_{123}$ . In the particular case where the matrix elements  $\rho_{ij}$  are all reals, we have  $K_{12} = K_{21} = 0$  and the eigenvalues  $k_1, k_2$  and  $k_3$  (52) of the matrix  $K$  coincide respectively with  $K_{11}, K_{22}$  and  $K_{33}$ . In other hand, if one ignores the qubit 3, the matrix elements (63) reduces to ones of two qubit  $X$  states and it simply verified that one recovers the results (36).

### 3.2.2 States of type $\sigma_{123}$

Similarly, for states of type  $\sigma_{123}$ , we write the matrix density (15) as follows

$$\sigma_{123} = \frac{1}{8} \left[ \mathcal{T}_{000} \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \mathcal{T}_{300} \sigma_3 \otimes \sigma_0 \otimes \sigma_0 + \sum_{(\beta, \gamma) \neq (0,0)} \mathcal{T}_{0\beta\gamma} \sigma_0 \otimes \sigma_\beta \otimes \sigma_\gamma + \sum_i \sum_{(\beta, \gamma) \neq (0,0)} \mathcal{T}_{i\beta\gamma} \sigma_i \otimes \sigma_\beta \otimes \sigma_\gamma \right] \quad (64)$$

Identifying the coefficients  $T_{\alpha\beta\gamma}$  occurring in (40) with  $\mathcal{T}_{\alpha\beta\gamma}$ , one obtains the corresponding matrix  $K$  (51) whose elements determine the geometric measure of quantum discord. Explicitly, we have

$$K_{kl} = \sum_{i=1,2} \sum_{j=0,3} \mathcal{T}_{kij} \mathcal{T}_{lij} + \mathcal{T}_{kji} \mathcal{T}_{lji} \quad (65)$$

for  $k, l = 1, 2$ , and

$$K_{33} = \sum_{i=0,3} \sum_{j=0,3} \mathcal{T}_{3ij}^2 + \sum_{i=1,2} \sum_{j=1,2} \mathcal{T}_{3ij}^2. \quad (66)$$

They can be rewritten in terms of the bipartite correlations matrix  $T^{ij}$  associated with the two qubit density matrices  $\sigma^{01}, \sigma^{01}, \sigma^{10}$  and  $\sigma^{11}$  given by (21) and (23). Indeed, using the relations (26) and (27), one shows that the diagonal elements are given by

$$K_{11} = 2[(T_{11}^{00})^2 + (T_{11}^{11})^2] + 2[(T_{12}^{00})^2 + (T_{12}^{11})^2] + 4|T_{10}^{01}|^2 + 4|T_{13}^{01}|^2 \quad (67)$$

$$K_{22} = 2[(T_{21}^{00})^2 + (T_{21}^{11})^2] + 2[(T_{22}^{00})^2 + (T_{22}^{11})^2] + 4|T_{20}^{01}|^2 + 4|T_{23}^{01}|^2 \quad (68)$$

$$K_{33} = 2[(T_{30}^{00})^2 + (T_{30}^{11})^2] + 2[(T_{33}^{00})^2 + (T_{33}^{11})^2] + 4|T_{31}^{01}|^2 + 4|T_{32}^{01}|^2 \quad (69)$$

where we have used the relation  $\overline{T_{\alpha,\beta}^{01}} = T_{\alpha,\beta}^{10}$ . The non zero off-diagonal element  $K_{12}$  rewrites

$$\begin{aligned} K_{12} = K_{21} &= 2(T_{21}^{00} T_{11}^{00} + T_{21}^{11} T_{11}^{11}) + 2(T_{22}^{00} T_{12}^{00} + T_{22}^{11} T_{12}^{11}) \\ &+ 2(\overline{T_{20}^{01}} T_{10}^{01} + T_{20}^{01} \overline{T_{10}^{01}}) + 2(\overline{T_{23}^{01}} T_{13}^{01} + T_{23}^{01} \overline{T_{13}^{01}}). \end{aligned} \quad (70)$$

Finally, using the relations (21) and (23), one gets

$$K_{11} = 8[|\sigma_{41} + \sigma_{23}|^2 + |\sigma_{85} + \sigma_{67}|^2] + 4[|\sigma_{17} + \sigma_{35} + \sigma_{28} + \sigma_{46}|^2 + |\sigma_{17} + \sigma_{35} - \sigma_{28} - \sigma_{46}|^2], \quad (71)$$

$$K_{22} = 8[|\sigma_{41} - \sigma_{23}|^2 + |\sigma_{85} - \sigma_{67}|^2] + 4[|\sigma_{17} - \sigma_{35} + \sigma_{28} - \sigma_{46}|^2 + |\sigma_{17} - \sigma_{35} - \sigma_{28} + \sigma_{46}|^2], \quad (72)$$

$$K_{33} = 4 \left[ (\sigma_{11} - \sigma_{33})^2 + (\sigma_{22} - \sigma_{44})^2 + (\sigma_{55} - \sigma_{77})^2 + (\sigma_{66} - \sigma_{88})^2 + |\sigma_{16} - \sigma_{38} - \sigma_{47} + \sigma_{25}|^2 + |\sigma_{16} - \sigma_{38} + \sigma_{47} - \sigma_{25}|^2 \right], \quad (73)$$



and

$$K_{12} = -16 \left[ |\sigma_{23}| |\sigma_{14}| \sin(\alpha_{23} + \alpha_{14}) + |\sigma_{58}| |\sigma_{67}| \sin(\alpha_{58} + \alpha_{67}) + |\sigma_{35}| |\sigma_{17}| \sin(\alpha_{17} - \alpha_{35}) + |\sigma_{28}| |\sigma_{46}| \sin(\alpha_{28} - \alpha_{46}) \right] \quad (74)$$

where  $\alpha_{ij} = \frac{\sigma_{ij}}{|\sigma_{ij}|}$  for  $i < j$ . Substituting the quantities (71), (72), (73) and (74) in the expressions (52), we have the geometric discord (53) in terms of matrix elements of  $\sigma_{123}$  (15). In the special situation where all the entries of the density matrix  $\sigma_{123}$  are reals, we have  $k_1 = K_{11}$ ,  $k_2 = K_{22}$  and  $k_3 = K_{33}$ .

## 4 Monogamy of geometric discord in three-qubit $X$ states

The quantum correlation can be transferred between the components of a quantum system comprising many parties. This shareability is however subject to the monogamy relation which is given for a three-qubit system by

$$Q_{1|23} \geq Q_{1|2} + Q_{2|3}$$

where  $Q$  denotes a measure of pairwise quantum correlation in the system. This inequality means that the amount of quantum correlation shared between the qubits 1 and 2 restricts the possible amount of quantum correlation between the qubits 2 and 3 so that the sum is always less than the total bipartite correlation between the qubit 1 and the subsystem containing the qubits 2 and 3. This important property was originally proposed by Coffman, Kundo and Wootters in 2001 [36] for squared concurrence and extended since then to other correlation quantifiers such as entanglement of formation [37, 38], quantum discord [39, 40, 41, 42, 43] and its geometric variant [44]. In particular, the geometric discord was proven to follow the monogamy property on all pure three-qubit states. Here, we shall investigate the distribution among the three qubits in the mixed states of type  $\rho_{123}$  (3) and  $\sigma_{123}$  (14).

### 4.1 Monogamy conditions

We consider first the states of type (3). The corresponding reduced matrices  $\rho_{12} = \text{Tr}_3 \rho_{123}$  and  $\rho_{13} = \text{Tr}_2 \rho_{123}$  are

$$\rho_{12} = \begin{pmatrix} \rho_{11} + \rho_{55} & 0 & 0 & \rho_{14} + \rho_{58} \\ 0 & \rho_{22} + \rho_{66} & \rho_{23} + \rho_{67} & 0 \\ 0 & \rho_{32} + \rho_{76} & \rho_{33} + \rho_{77} & 0 \\ \rho_{41} + \rho_{85} & 0 & 0 & \rho_{44} + \rho_{88} \end{pmatrix} \quad (75)$$

$$\rho_{13} = \begin{pmatrix} \rho_{11} + \rho_{22} & \rho_{15} + \rho_{26} & 0 & 0 \\ \rho_{51} + \rho_{62} & \rho_{55} + \rho_{66} & 0 & 0 \\ 0 & 0 & \rho_{33} + \rho_{44} & \rho_{37} + \rho_{48} \\ 0 & 0 & \rho_{73} + \rho_{84} & \rho_{77} + \rho_{88} \end{pmatrix}. \quad (76)$$

The reduced two qubit states  $\rho_{12}$  (75) is  $X$ -shaped. The bipartite geometric discord can be derived using the results (36). Therefore, the bipartite quantum correlation in the state  $\rho_{12}$ , as measured by

Hilbert-Schmidt distance, is

$$D_g(\rho_{12}) = \frac{1}{4}(q_2 + \min(q_1 + q_3)) \quad (77)$$

where

$$\begin{aligned} q_1 &= 4(|\rho_{14} + \rho_{58}| + |\rho_{23} + \rho_{67}|)^2 \\ q_2 &= 4(|\rho_{14} + \rho_{58}| - |\rho_{23} + \rho_{67}|)^2 \\ q_3 &= 2[(\rho_{11} + \rho_{55} - \rho_{33} - \rho_{77})^2 + (\rho_{22} + \rho_{66} - \rho_{44} - \rho_{88})^2]. \end{aligned} \quad (78)$$

The state  $\rho_{13}$  (76) is classically correlated. The quantum correlation between the qubits 1 and 3 is zero. This is easily verified using the prescription described previously to get the discord in an arbitrary two qubit state. In this special case, the eigenvalues of the analogue of the matrix  $K$  (35) are

$$\begin{aligned} p_1 &= p_2 = 0 \\ p_3 &= 2[(\rho_{11} + \rho_{22} - \rho_{33} - \rho_{44})^2 + (\rho_{55} + \rho_{66} - \rho_{77} - \rho_{88})^2] \end{aligned}$$

which implies that the geometric discord is indeed zero:

$$D_g(\rho_{13}) = 0. \quad (79)$$

It follows that the geometric discord in the three-qubit states  $\rho_{123}$  (3) is monogamous when

$$D_g(\rho_{1|23}) \geq D_g(\rho_{12}) \quad (80)$$

where  $D_g(\rho_{1|23})$  and  $D_g(\rho_{12})$  are respectively given by (53) and (77).

Analogously, for the states of type  $\sigma_{123}$  (14), the reduced two qubit states are

$$\sigma_{12} = \begin{pmatrix} \sigma_{11} + \sigma_{55} & 0 & 0 & \sigma_{14} + \sigma_{58} \\ 0 & \sigma_{22} + \sigma_{66} & \sigma_{23} + \sigma_{67} & 0 \\ 0 & \sigma_{32} + \sigma_{76} & \sigma_{33} + \sigma_{77} & 0 \\ \sigma_{41} + \sigma_{85} & 0 & 0 & \sigma_{44} + \sigma_{88} \end{pmatrix} \quad (81)$$

$$\sigma_{13} = \begin{pmatrix} \sigma_{11} + \sigma_{22} & 0 & 0 & \sigma_{17} + \sigma_{28} \\ 0 & \sigma_{55} + \sigma_{66} & \sigma_{53} + \sigma_{64} & 0 \\ 0 & \sigma_{35} + \sigma_{46} & \sigma_{33} + \sigma_{44} & 0 \\ \sigma_{71} + \sigma_{82} & 0 & 0 & \sigma_{77} + \sigma_{88} \end{pmatrix}. \quad (82)$$

The two qubit density matrices  $\sigma_{12}$  and  $\sigma_{13}$  are  $X$  shaped. It follows that the geometric measure of pairwise quantum discord arises directly from the results (36) modulo the appropriate substitutions. Accordingly, for  $\sigma_{12}$ , the geometric quantum discord is

$$D_g(\sigma_{12}) = \frac{1}{4}\min(l_1 + l_2, l_3 + l_2) \quad (83)$$

where

$$l_1 = 4(|\sigma_{14} + \sigma_{58}| + |\sigma_{23} + \sigma_{67}|)^2$$

$$l_2 = 4(|\sigma_{14} + \sigma_{58}| - |\sigma_{23} + \sigma_{67}|)^2$$

$$l_3 = 2[(\sigma_{11} + \sigma_{55} - \sigma_{33} - \sigma_{77})^2 + (\sigma_{22} + \sigma_{66} - \sigma_{44} - \sigma_{88})^2].$$

In the same way, for the subsystem described by  $\sigma_{13}$ , one gets

$$D_g(\sigma_{12}) = \frac{1}{4} \min(m_1 + m_2, m_3 + m_2) \quad (84)$$

where

$$m_1 = 4(|\sigma_{17} + \sigma_{28}| + |\sigma_{53} + \sigma_{64}|)^2$$

$$m_2 = 4(|\sigma_{17} + \sigma_{28}| - |\sigma_{53} + \sigma_{64}|)^2$$

$$m_3 = 2[(\sigma_{11} + \sigma_{22} - \sigma_{33} - \sigma_{44})^2 + (\sigma_{55} + \sigma_{66} - \sigma_{77} - \sigma_{88})^2].$$

The geometric discord satisfies the monogamy property when the entries of the density matrix  $\sigma_{123}$  satisfy the inequality

$$D_g(\sigma_{1|23}) \geq D_g(\sigma_{12}) + D_g(\sigma_{13}) \quad (85)$$

where the  $D_g(\sigma_{1|23})$  is evaluated from (53). To exemplify these results, we consider some special instances of mixed three-qubit states.

## 4.2 Some special mixed states

### 4.2.1 Mixed GHZ-states

We consider the mixed three-qubit GHZ state defined by

$$\rho_{\text{GHZ}} = \frac{p}{8} \mathbb{I} + (1 - p) |\text{GHZ}\rangle\langle\text{GHZ}| \quad (86)$$

where the pure GHZ-state is given by  $|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ . The states  $\rho_{\text{GHZ}}$  belong to the class of mixed three-qubit states of type  $\rho_{123}$  (3). Subsequently, using the expressions (63), it is simple to verify that the eigenvalues of the matrix  $K$  are

$$\lambda_1 = \lambda_2 = \lambda_3 = 2(1 - p)^2$$

and thus the geometric measure of the pairwise discord between the subsystems 1 and 23 is

$$D_g(\rho_{\text{GHZ}}) = \frac{1}{2}(1 - p)^2. \quad (87)$$

The maximal value of quantum correlation is reached for  $p = 0$  (pure GHZ state), and for  $p = 1$  the discord is vanishing as expected. To discuss the monogamy, we determine the pairwise geometric discord in the subsystems containing the qubits 1 – 2 and the qubits 1 – 3. We denote the associated states by  $\rho_{\text{GHZ}_{12}}$  and  $\rho_{\text{GHZ}_{23}}$  respectively. Using the results (77) and (79), one obtains

$$D_g(\rho_{\text{GHZ}_{12}}) = 0 \quad D_g(\rho_{\text{GHZ}_{13}}) = 0.$$

Using the result (87), one has

$$D_g(\rho_{\text{GHZ}}) \geq D_g(\rho_{\text{GHZ}_{12}}) + D_g(\rho_{\text{GHZ}_{13}}), \quad (88)$$

reflecting that the quantum discord in the states  $\rho_{\text{GHZ}}$ , as quantified by Hilbert-Schmidt norm, follows the monogamy constraint.

### 4.2.2 Mixed W-states

The second example deals with a special type of three-qubit states  $\sigma_{123}$  (14). They are given by

$$\sigma_W = \frac{p}{8} \mathbb{I} + (1-p) |W\rangle\langle W|. \quad (89)$$

in terms of the  $W$  state:  $|W\rangle = \frac{1}{\sqrt{3}}|100\rangle + |010\rangle + |001\rangle$ . Using the expressions (71)-(74), one gets

$$\lambda_1 = \lambda_2 = \frac{16}{9}(1-p)^2 \quad \lambda_3 = \frac{20}{9}(1-p)^2$$

and the geometric discord reads as

$$D_g(\sigma_W) = \frac{4}{9}(1-p)^2. \quad (90)$$

In other hand, from the equations (83) and (84), one has

$$D_g(\sigma_{W_{12}}) = D_g(\sigma_{W_{13}}) = \frac{1}{6}(1-p)^2. \quad (91)$$

where  $\rho_{W_{12}}$  and  $\rho_{W_{23}}$  are the two qubit states corresponding to the subsystems comprising the qubits 1-2 and 1-3 respectively. It is clear that

$$D_g(\rho_W) \geq D_g(\rho_{W_{12}}) + D_g(\rho_{W_{13}}). \quad (92)$$

The geometric measure of quantum discord in the states  $\sigma_W$  satisfies the monogamy condition.

### 4.2.3 Three-qubit state of Bell type

Finally, we consider the three-qubit

$$\rho_B = \frac{1}{8} \left( \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \sum_{i=0}^3 c_i \sigma_i \otimes \sigma_i \otimes \sigma_i \right). \quad (93)$$

which can be viewed as the extended version of two-qubit Bell state. The state  $\rho_B$  has non vanishing matrix elements only along the diagonal and off diagonal. Indeed, in the computational basis, it writes

$$\rho_B = \frac{1}{8} \begin{pmatrix} 1+c_3 & 0 & 0 & 0 & 0 & 0 & 0 & c_1+ic_2 \\ 0 & 1-c_3 & 0 & 0 & 0 & 0 & c_1-ic_2 & 0 \\ 0 & 0 & 1-c_3 & 0 & 0 & c_1-ic_2 & 0 & 0 \\ 0 & 0 & 0 & 1+c_3 & c_1+ic_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_1-ic_2 & 1-c_3 & 0 & 0 & 0 \\ 0 & 0 & c_1+ic_2 & 0 & 0 & 1+c_3 & 0 & 0 \\ 0 & c_1+ic_2 & 0 & 0 & 0 & 0 & 1+c_3 & 0 \\ c_1-ic_2 & 0 & 0 & 0 & 0 & 0 & 0 & 1+c_3 \end{pmatrix}. \quad (94)$$

From equations (63), one has

$$K_{11} = c_1^2 \quad K_{22} = c_2^2 \quad K_{33} = c_3^2 \quad K_{21} = K_{21} = 0$$

and the geometric discord in the bipartition 1|23 is

$$D_g(\rho_B) = \frac{1}{8}(c_1^2 + c_2^2 + c_3^2 - c^2) \quad (95)$$

where  $c^2 = \max(c_1^2, c_2^2, c_3^2)$ . It is remarkable that the reduced two qubit states given by

$$\rho_{B_{12}} = \rho_{B_{13}} = \frac{1}{4}\sigma_0 \otimes \sigma_0$$

do not present quantum correlations when measured by the Hilbert-Schmidt distance (*i.e.*,  $D_g(\rho_{B_{12}}) = D_g(\rho_{B_{13}}) = 0$ ). The quantum  $D_g(\rho_B)$  is always non negative and therefore the geometric discord in the states  $\rho_B$  is monogamous.

## 5 Concluding remarks

In this work, we have investigated the analytical derivation of quantum correlations in mixed states describing quantum systems comprising three qubits. We have deliberately considered the square norm (Hilbert-Schmidt distance) instead of entropic based quantifiers. In fact, despite the information meaning of based entropy measures, determining explicit expressions of quantum correlations requires optimization procedures that are in general very complicated to achieve even in two qubit systems. In this respect, the geometric quantifiers are advantageous in obtaining closed computable expressions of the information contained in a tripartite quantum system. In this picture, through the geometrized variant of quantum discord, we characterized the bipartite quantum correlations in mixed three-qubit states and their analytic expressions are explicitly derived for two families of generalized three-qubit  $X$ - states. In addition, we have determined the explicit Fano-Bloch expressions of classically correlated (zero discord) states. In other hand, we have studied the monogamy property and the shareability limitations of geometric quantum discord for two kinds of generalized three-qubit  $X$  states. To exemplify our results, we discussed the monogamy property in mixed three-qubit states of  $W$ ,  $GHZ$  and  $Bell$  types.

Finally, it is interesting to note that the results presented in this paper can be generalized to quantum systems comprising more qubits and can be used to derive the total amount of all pairwise quantum correlations existing in a multi-qubit system (see for instance [44, 45, 46]). On the other hand, our results are applicable in investigating quantum decoherence in mixed three-qubit systems [49]. Further study in this direction might be worthwhile.

## References

- [1] M.A. Nielsen and I.L. Chuang: *Quantum Computation and Quantum Information*, Cambridge University Press, Cambridge (2000).
- [2] R. Horodecki, P. Horodecki, M. Horodecki and K. Horodecki: *Rev. Mod. Phys.* **81**, 865 (2009).

- [3] O. Ghne and G. Tth: *Phys. Rep.* **474**, 1 (2009).
- [4] V. Vedral: *Rev. Mod. Phys.* **74**, 197 (2002).
- [5] K. Modi, A. Brodutch, H. Cable, T. Paterek and V. Vedral: *Rev. Mod. Phys.* **84**, 1655 (2012).
- [6] W.K. Wootters: *Phys. Rev. Lett.* **80**, 2245 (1998); W.K. Wootters, *Quant. Inf. Comp.* **1**, 27 (2001).
- [7] S. Hill and W.K. Wootters: *Phys. Rev. Lett.* **78**, 5022 (1997).
- [8] H. Ollivier and W.H. Zurek: *Phys. Rev. Lett.* **88**, 017901 (2001).
- [9] L. Henderson and V. Vedral: *J. Phys. A* **34**, 6899 (2001); V. Vedral, *Phys. Rev. Lett.* **90**, 050401 (2003); J. Maziero, L.C. Celri, R.M. Serra and V. Vedral: *Phys. Rev. A* **80**, 044102 (2009).
- [10] B. Dakic, V. Vedral and C. Brukner: *Phys. Rev. Lett.* **105**, 190502 (2010).
- [11] S.Vinjanampathy and A.R.P Rau: *J. Phys. A: Math. Theor.* **45**, 095303 (2012).
- [12] T. Yu and J. H. Eberly: *Quant. Inf. Comp.* **7**, 459 (2007); *Phys. Rev. Lett.* **93** (2004) 140404; *ibid* **97**, 140403 (2006).
- [13] R. Dillenschneider: *Phys. Rev. B* **78**, 22413 (2008).
- [14] S. Luo: *Phys. Rev. A* **77**, 042303 (2008).
- [15] M.S. Sarandy: *Phys. Rev. A* **80**, 022108 (2009).
- [16] T. Werlang, S. Souza, F.F. Fanchini and C.J. Villas Boas: *Phys. Rev. A* **80**, 024103 (2009).
- [17] L. Jakobczyk and A. Jamroz: *Phys. Lett. A* **333**, 35 (2004).
- [18] M. Franca Santos, P. Milman, L. Davidovich and N. Zagury: *Phys. Rev. A* **73**, 040305 (2006).
- [19] A. Jamroz: *J. Phys. A: Math. Gen.* **39**, 727 (2006).
- [20] M. Ikram, F.L. Li and M.S. Zubairy: *Phys. Rev. A* **75**, 062336 (2007).
- [21] A. Al-Qasimi and D.F.V. James: *Phys. Rev. A* **77**, 012117 (2007).
- [22] A. R. P. Rau, M. Ali and G. Alber: *Eur. Phys. Lett* **82**, 40002 (2008).
- [23] X. Cao and H. Zheng: *Phys. Rev. A* **77**, 022320 (2008).
- [24] C.E. Lopez, G. Romero, F. Castra, E. Solano and J.C. Retamal: *Phys. Rev. Lett.* **101**, 080503 (2008).
- [25] M. Ali, G. Alber and A.R.P. Rau: *J. Phys. B: At. Mol. Opt. Phys.* **42**, 025501 (2009); M. Ali, A.R.P. Rau and G. Alber: *Phys. Rev. A* **81**, 042105 (2019).

- [26] M. Daoud and R. Ahl Laamara: *J. Phys. A: Math. Theor.* **45**, 325302 (2012).
- [27] M. Daoud and R. Ahl Laamara: *Phys. Lett. A* **376**, 2361 (2012).
- [28] A.R.P. Rau: *Phys. Rev. A* **79**, 042323 (2009).
- [29] A.R.P. Rau, G. Selvaraj and D. Uskov: *Phys. Rev. A* **71**, 062316 (2005).
- [30] D. Uskov and A.R.P. Rau: *Phys. Rev. A* **74**, 030304 (R) (2005) ; *ibid* **78**, 022331 (2008).
- [31] F.J.M. van de Ven and C.W. Hilbers: *J. Magn. Reson.* **54**, 512 (1983).
- [32] R.F. Werner: *Phys. Rev. A* **40**, 4277 (1989).
- [33] J. Zhang, J. Vala, S. Sastry and K.B. Whaley: *Phys. Rev. A* **67**, 042313 (2003).
- [34] T. Beth, D. Jungnickel and H. Lenz: *Design Theory*, Vols. 1 and 2, Encyclopaedia of Mathematics, Vol. 69 (Bibl. Inst., Zürich, 1985; Cambridge University Press, Cambridge 1993).
- [35] G. M. Dixon: *Division Algebras: Octonions, Quaternions, Complex Numbers and the Algebraic Design of Physics*, Vol. 290 of Mathematics and its Applications, Kluwer, Dordrecht (1994); J. C. Baez: *Bull. Am. Math. Soc.* **39**, 145 (2002).
- [36] V. Coffman, J. Kundu and W.K. Wootters, *Phys. Rev. A* **61**, 052306 (2000).
- [37] G. Adesso and F. Illuminati: *New J. Phys.* **8**, 15 (2006).
- [38] T.Hiroshima, G. Adesso and F. Illuminati: *Phys. Rev. Lett.* **98**, 050503 (2007).
- [39] G.L. Giorgi: *Phys. Rev. A* **84**, 054301 (2011).
- [40] R. Prabhu, A.K. Pati, A.S. De and U. Sen: *Phys. Rev. A* **86**, 052337 (2012).
- [41] Sudha, A.R. Usha Devi and A.K. Rajagopal: *Phys. Rev. A* **85**, 012103 (2012).
- [42] M. Allegra, P. Giorda and A. Montorsi: *Phys. Rev. B* **84**, 245133 (2011).
- [43] X.-J. Ren and H. Fan: *Quant. Inf. Comp.* **13**, 0469 (2013).
- [44] A. Streltsov, G. Adesso, M. Piani and D. Bruss: *Phys. Rev. Lett.* **109**, 050503 (2012).
- [45] M. Daoud, R. Ahl Laamara and W. Kaydi: *J. Phys. A: Math. Theor.* **46**, 395302 (2013).
- [46] M. Daoud, R. Ahl Laamara and R. Essaber: *Inter. J. Quant. inf.* **11**, 1350057 (2013).
- [47] M. Daoud. R. Ahl Laamara and S. Seddik: *Inter. J. Mod. Phys. B* **29**, 1550124 (2015).
- [48] X. Wang and B.C. Sanders: *Phys. Rev. A* **68**, 012101 (2003).
- [49] J. Zhou and H. Guo: *Phys. Rev. A* **87**, 062315 (2013).