Hilbert-Schmidt measure of pairwise quantum discord in three qubit X states

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Abstract

The Hilbert-Schmidt distance between a mixed three qubits 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 ressource 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, 13, 14, 15, 16, 17, 18, 19, 20, 21, 23, 24, 25, 26, 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, for a tripartite system $1-2-3$, the sum of quantum correlations $Q_{1|2}$ (the shared correlation Q between 1 and 2) and $Q_{1|3}$ (the shared correlation Q 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 [45, 44, 46] do not follows 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 specify three qubit mixed states are given. Concluding remarks close this paper.

2　Three-qubit X-states

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

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

where the Fano-Bloch parameters are given by $T_{\alpha\beta} = \text{Tr}(\rho_{12}\sigma_\alpha \otimes \sigma_\beta)$ and σ_α are the Pauli matrices. The symmetry of two qubit systems is fully characterized by the algebra $su(4)$ spanned by the 4×4 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 $su(2) \times u(1) \times su(2) \subset su(4)$

spanned by seven linearly independent generators. Specifically, X states can be written as

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

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 ρ_{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

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

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

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

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

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

with $\mathcal{R}_{000} = 1$ ($\text{Tr}(\rho_{123}) = 1$). The operators σ_α stands for Pauli basis with σ_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 (α, β, γ) belonging to the following set of triplets

$$(000), (001), (002), (003), (030), (031), (032), (033)$$

$$(110), (111), (112), (113), (120), (121), (122), (123)$$

$$(210), (211), (212), (213), (220), (221), (222), (223)$$

$$(300), (301), (302), (303), (330), (331), (332), (333). \tag{5}$$

Accordingly, the state (4) expand as

$$\rho_{123} = \frac{1}{8}\left[\mathcal{R}_{000}\sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \sum_i \left(\mathcal{R}_{i00}\ \sigma_i \otimes \sigma_0 \otimes \sigma_0 + \mathcal{R}_{0i0}\ \sigma_0 \otimes \sigma_i \otimes \sigma_0 + \mathcal{R}_{00i}\ \sigma_0 \otimes \sigma_0 \otimes \sigma_i \right) \right.$$

$$\left. + \sum_{ij} \left(\mathcal{R}_{ij0}\ \sigma_i \otimes \sigma_j \otimes \sigma_0 + \mathcal{R}_{i0j}\ \sigma_i \otimes \sigma_0 \otimes \sigma_j + \mathcal{R}_{0ij}\ \sigma_0 \otimes \sigma_i \otimes \sigma_j \right) + \sum_{ijk} \mathcal{R}_{ijk}\ \sigma_i \otimes \sigma_j \otimes \sigma_k \right], \tag{6}$$

in terms of 32 operators which span the subalgebra $su(2) \otimes u(1) \otimes su(2) \otimes u(1) \otimes su(2) \otimes u(1) \otimes su(2)$ of the full symmetry algebra $su(8)$ 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 ρ_{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

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

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

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

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 ρ^{ij} (8) are

$$\rho^{ij} = \frac{1}{4}\sum_{\alpha\beta} R^{ij}_{\alpha\beta}\sigma_\alpha \otimes \sigma_\beta \tag{9}$$

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

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

are given by

$$R_{00}^{ij} = 1$$

$$R_{30}^{ij} = \rho_{1+4i\ 1+4j} + \rho_{2+4i\ 2+4j} - \rho_{3+4i\ 3+4j} - \rho_{4+4i\ 4+4j}$$

$$R_{03}^{ij} = \rho_{1+4i\ 1+4j} - \rho_{2+4i\ 2+4j} + \rho_{3+4i\ 3+4j} - \rho_{4+4i\ 4+4j}$$

$$R_{11}^{ij} = \rho_{1+4i\ 4+4j} + \rho_{4+4i\ 1+4j} + \rho_{2+4i\ 3+4j} + \rho_{3+4i\ 2+4j}$$

$$R_{12}^{ij} = i(\rho_{1+4i\ 4+4j} - \rho_{4+4i\ 1+4j} - \rho_{2+4i\ 3+4j} + \rho_{3+4i\ 2+4j})$$

$$R_{21}^{ij} = i(\rho_{1+4i\ 4+4j} - \rho_{4+4i\ 1+4j} + \rho_{2+4i\ 3+4j} - \rho_{3+4i\ 2+4j})$$

$$R_{22}^{ij} = \rho_{2+4i\ 3+4j} + \rho_{3+4i\ 2+4j} - \rho_{1+4i\ 4+4j} - \rho_{4+4i\ 1+4j}$$

$$R_{33}^{ij} = \rho_{1+4i\ 1+4j} - \rho_{2+4i\ 2+4j} - \rho_{3+4i\ 3+4j} + \rho_{4+4i\ 4+4j}). \tag{10}$$

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

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

and similarly, we rewrite (6) as

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

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

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

$$\mathcal{R}_{\alpha\beta 3} = R_{\alpha\beta}^{--} = R_{\alpha\beta}^{00} - R_{\alpha\beta}^{11}$$

$$\mathcal{R}_{\alpha\beta 1} = R_{\alpha\beta}^{+-} = R_{\alpha\beta}^{01} + R_{\alpha\beta}^{10}$$

$$\mathcal{R}_{\alpha\beta 2} = R_{\alpha\beta}^{-+} = iR_{\alpha\beta}^{01} - iR_{\alpha\beta}^{10}. \tag{13}$$

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 σ_{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 σ_{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 $su(2) \otimes u(1) \otimes su(2) \otimes u(1) \otimes su(2) \otimes u(1) \otimes su(2)$. In the Fano-Bloch representation, the matrix density (14) expands as

$$\sigma_{123} = \frac{1}{8} \Bigg[\mathcal{T}_{000} \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + \sum_i \left(\mathcal{T}_{i00} \; \sigma_i \otimes \sigma_0 \otimes \sigma_0 + \mathcal{T}_{0i0} \; \sigma_0 \otimes \sigma_i \otimes \sigma_0 + \mathcal{T}_{00i} \; \sigma_0 \otimes \sigma_0 \otimes \sigma_i \right)$$

$$+ \sum_{ij} \left(\mathcal{T}_{ij0} \; \sigma_i \otimes \sigma_j \otimes \sigma_0 + \mathcal{T}_{i0j} \; \sigma_i \otimes \sigma_0 \otimes \sigma_j + \mathcal{T}_{0ij} \; \sigma_0 \otimes \sigma_i \otimes \sigma_j \right) + \sum_{ijk} \mathcal{T}_{ijk} \; \sigma_i \otimes \sigma_j \otimes \sigma_k \Bigg] \tag{15}$$

where the the matrix correlation elements are

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

with $\mathcal{T}_{000} = 1$ ($\mathrm{Tr}(\sigma_{123}) = 1$). 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

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

$$(101), (102), (110), (113), (120), (123), (131), (132)$$

$$(201), (202), (210), (213), (220), (223), (231), (232)$$

$$(300), (303), (311), (312), (321), (322), (330), (333). \tag{16}$$

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 σ^{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 σ^{ii} are

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

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

$$T^{ii}_{00} = 1$$

$$T^{ii}_{30} = \sigma_{1+4i\ 1+4i} + \sigma_{2+4i\ 2+4i} - \sigma_{3+4i\ 3+4i} - \sigma_{4+4i\ 4+4i}$$

$$T^{ii}_{03} = \sigma_{1+4i\ 1+4i} - \sigma_{2+4i\ 2+4i} + \sigma_{3+4i\ 3+4i} - \sigma_{4+4i\ 4+4i}$$

$$T^{ii}_{11} = \sigma_{1+4i\ 4+4i} + \sigma_{4+4i\ 1+4i} + \sigma_{2+4i\ 3+4i} + \sigma_{3+4i\ 2+4i}$$

$$T^{ii}_{12} = i(\sigma_{1+4i\ 4+4i} - \sigma_{4+4i\ 1+4i} - \sigma_{2+4i\ 3+4i} + \sigma_{3+4i\ 2+4i})$$

$$T^{ii}_{21} = i(\sigma_{1+4i\ 4+4i} - \sigma_{4+4i\ 1+4i} + \sigma_{2+4i\ 3+4i} - \sigma_{3+4i\ 2+4i})$$

$$T^{ii}_{22} = \sigma_{2+4i\ 3+4i} + \sigma_{3+4i\ 2+4i} - \sigma_{1+4i\ 4+4i} - \sigma_{4+4i\ 1+4i}$$

$$T^{ii}_{33} = \sigma_{1+4i\ 1+4i} - \sigma_{2+4i\ 2+4i} - \sigma_{3+4i\ 3+4i} + \sigma_{4+4i\ 4+4i}). \tag{21}$$

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

$$\sigma^{ij} = \frac{1}{4} \sum_{\alpha\beta} T^{ij}_{\alpha\beta}\ \sigma_\alpha \otimes \sigma_\beta \qquad i \neq j \tag{22}$$

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

$$T^{ij}_{01} = \sigma_{2+4i\ 1+4j} + \sigma_{1+4i\ 2+4j} + \sigma_{4+4i\ 3+4j} + \sigma_{3+4i\ 4+4j}$$

$$T^{ij}_{02} = i(-\sigma_{2+4i\ 1+4j} + \sigma_{1+4i\ 2+4j} - \sigma_{4+4i\ 3+4j} + \sigma_{3+4i\ 4+4j})$$

$$T^{ij}_{10} = \sigma_{1+4i\ 3+4j} + \sigma_{3+4i\ 1+4j} + \sigma_{2+4i\ 4+4j} + \sigma_{4+4i\ 2+4j}$$

$$T_{13}^{ij} = \sigma_{1+4i\ 3+4j} + \sigma_{3+4i\ 1+4j} - \sigma_{2+4i\ 4+4j} - \sigma_{4+4i\ 2+4j}$$

$$T_{20}^{ij} = i(\sigma_{1+4i\ 3+4j} - \sigma_{3+4i\ 1+4j} + \sigma_{2+4i\ 4+4j} - \sigma_{4+4i\ 2+4j})$$

$$T_{23}^{ij} = i(\sigma_{1+4i\ 3+4j} - \sigma_{3+4i\ 1+4j} - \sigma_{2+4i\ 4+4j} + \sigma_{4+4i\ 2+4j})$$

$$T_{31}^{ij} = \sigma_{1+4i\ 2+4j} + \sigma_{2+4i\ 1+4j} - \sigma_{3+4i\ 4+4j} - \sigma_{4+4i\ 3+4j})$$

$$T_{32}^{ij} = i(\sigma_{1+4i\ 2+4j} - \sigma_{2+4i\ 1+4j} - \sigma_{3+4i\ 4+4j} + \sigma_{4+4i\ 3+4j}). \tag{23}$$

Using (17), one obtains

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

The three qubit state (15) rewrites also as

$$\sigma_{123} = \frac{1}{8}\sum_{\alpha\beta}\left[\mathcal{T}_{\alpha\beta0}\ \sigma_\alpha \otimes \sigma_\beta \otimes \sigma_0 + \mathcal{T}_{\alpha\beta1}\ \sigma_\alpha \otimes \sigma_\beta \otimes \sigma_1 + \mathcal{T}_{\alpha\beta2}\ \sigma_\alpha \otimes \sigma_\beta \otimes \sigma_2 + \mathcal{T}_{\alpha\beta3}\ \sigma_\alpha \otimes \sigma_\beta \otimes \sigma_3\right] \tag{25}$$

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

$$\mathcal{T}_{\alpha\beta0} = T_{\alpha\beta}^{++} = T_{\alpha\beta}^{00} + T_{\alpha\beta}^{11}$$

$$\mathcal{T}_{\alpha\beta3} = T_{\alpha\beta}^{--} = T_{\alpha\beta}^{00} - T_{\alpha\beta}^{11} \tag{26}$$

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

$$\mathcal{T}_{\alpha\beta1} = T_{\alpha\beta}^{+-} = T_{\alpha\beta}^{01} + T_{\alpha\beta}^{10}$$

$$\mathcal{T}_{\alpha\beta2} = T_{\alpha\beta}^{-+} = iT_{\alpha\beta}^{01} - iT_{\alpha\beta}^{10} \tag{27}$$

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

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 quantunmness 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

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

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 ρ_{12} and its closest classical-quantum state presenting zero discord [10]

$$D_{\mathrm{g}}(\rho_{12}) = \min_{\chi_{12}} ||\rho_{12} - \chi_{12}||^2 \tag{29}$$

where the Hilbert-Schmidt norm is defined by $||X||^2 = \mathrm{Tr}(X^\dagger X)$ 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

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

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 ρ_i^2 ($i = 1, 2$) is the marginal density of the qubit 2. The classically correlated states χ_{12} can also be written as

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

where

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

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

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

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

$$t = e_3 T_{30}$$

$$(s_+)_1 = 0 \quad (s_+)_2 = 0 \quad (s_+)_3 = T_{03}$$

$$(s_-)_i = \sum_{j=1}^{3} e_j T_{ji}. \tag{33}$$

Inserting these solutions in (32), one has

$$||\rho_{12} - \chi_{12}||^2 = \frac{1}{4}\left[\mathrm{Tr}K - \vec{e}^{\,t}K\vec{e}\right] \tag{34}$$

where the matrix K is defined by

$$K = xx^\dagger + TT^\dagger \tag{35}$$

with

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

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 λ_1, λ_2 and λ_3 the eigenvalues of the matrix K (35) corresponding to the X state (2) or equivalently (28). They are given by

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

To get the minimal value of the Hilbert-Schmidt distance (34) and subsequently the amount of geometric quantum discord, one compares λ_1, λ_2 and λ_3. As λ_1 is always greater than λ_2, the largest eigenvalue $\lambda_{\max}$ is λ_1 or λ_3. It follows that the geometric discord is given by

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

To write down the explicit expressions of the closest classical state χ_{12} to ρ_{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 ρ_{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

$$\chi_{12}^3 = \frac{1}{4}\left[\sigma_0 \otimes \sigma_0 + T_{30}\ \sigma_3 \otimes \sigma_0 + T_{03}\ \sigma_0 \otimes \sigma_3 + T_{33}\ \sigma_3 \otimes \sigma_3\right] \tag{38}$$

In the second situation, the eigenvector corresponding to λ_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

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

where

$$\tilde{T}_{11} = \cos\frac{\phi}{2}(\cos\frac{\phi}{2}T_{11} - \sin\frac{\phi}{2}T_{21}) \qquad \tilde{T}_{12} = \cos\frac{\phi}{2}(\cos\frac{\phi}{2}T_{12} - \sin\frac{\phi}{2}T_{22})$$

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

As we already mentioned, the geometric quantifiers of quantum correlations in bipartite systems can be extended to embrace three qubits 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 ρ_{123} (3) and σ_{123} (14). The algebraic structures of both three qubit density matrices offer many simplification in quantifying geometric quantum discord. To deal with the states ρ_{123} (3) and σ_{123} (14) in a common framework, it is interesting to note that ρ_{123} as well as σ_{123} have a similar Fano-Bloch representation. That is

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

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 ϱ_{123} of type ρ_{123} (3)(resp. σ_{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

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

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

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

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

$$\chi_{1|23} = \frac{1}{8}\left[\sigma_0\otimes\sigma_0\otimes\sigma_0 + \sum_{i=1}^{3} te_i \;\; \sigma_i\otimes\sigma_0\otimes\sigma_0 \right.$$

$$\left. + \sum_{(\alpha,\beta)\neq(0,0)} (s_+)_{\alpha,\beta}\,\sigma_0\otimes\sigma_\alpha\otimes\sigma_\beta + \sum_{i=1}^{3}\sum_{(\alpha,\beta)\neq(0,0)} e_i(s_-)_{\alpha,\beta}\,\sigma_i\otimes\sigma_\alpha\otimes\sigma_\beta \right] \tag{42}$$

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

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

$$||\varrho_{1|23}-\chi_{1|23}||^2 = \frac{1}{8}\left[(t^2-2te_3T_{300}+T_{300}^2) + \sum_{(\alpha,\beta)\neq(0,0)} (T_{0\alpha\beta}-(s_+)_{\alpha,\beta})^2 + \sum_{i=1}^{3}\sum_{(\alpha,\beta)\neq(0,0)} (T_{i\alpha\beta}-e_i(s_-)_{\alpha,\beta})^2 \right]. \tag{43}$$

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

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

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

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

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

$$||\varrho_{1|23} - \chi_{1|23}||^2 = \frac{1}{8}\left[||x||^2 + ||T||^2 - \vec{e}^{\,t}(xx^t + TT^t)\vec{e}\right] \tag{46}$$

in terms of the 3×1 matrix x defined by

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

and the 3×15 matrix given by

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

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

$$K = xx^t + TT^t. \tag{49}$$

It follows that the minimal value given by

$$D_{\text{g}}(\varrho_{1|23}) = \frac{1}{8}(k_1 + k_2 + k_3 - k_{\max}) \tag{50}$$

is the measure quantifying the pairwise quantum discord in the state ϱ_{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 ρ_{123} (3) as well as σ_{123} (14), the matrix K takes the form

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

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

$$k_1 = \frac{1}{2}(K_{11} + K_{22}) + \frac{1}{2}\sqrt{(K_{11} + K_{22})^2 - 4(K_{11}K_{22} - K_{12}K_{21})}$$

$$k_2 = \frac{1}{2}(K_{11} + K_{22}) - \frac{1}{2}\sqrt{(K_{11} + K_{22})^2 - 4(K_{11}K_{22} - K_{12}K_{21})}$$

$$k_3 = K_{33}. \tag{52}$$

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

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

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 ϱ_{123} with entries satisfying the condition $k_{\max} = k_1$, it is easy to verify that the maximal eigenvector is given by

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

and subsequently the closest classical states write

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

where

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

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

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

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 ρ_{123} and σ_{123}. This issue is discussed in what follows.

3.2.1 States of type ρ_{123}

For three qubit states ϱ_{123} (40) belonging to class of states of type (6), we have

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

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

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

and

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

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

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

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

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

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

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

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

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

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

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

$$\tag{63}$$

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 ρ_{123}. In the particular case where the matrix elements ρ_{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 σ_{123}

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

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

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

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

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

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

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

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

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

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

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

$$K_{12} = K_{21} = 2(T_{21}^{00}T_{11}^{00} + T_{21}^{11}T_{11}^{11}) + 2(T_{22}^{00}T_{12}^{00} + T_{22}^{11}T_{12}^{11})$$

$$+2(\overline{T_{20}^{01}}T_{10}^{01} + T_{20}^{01}\overline{T_{10}^{01}}) + 2(\overline{T_{23}^{01}}T_{13}^{01} + T_{23}^{01}\overline{T_{13}^{01}}). \tag{70}$$

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

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

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

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

and

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

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 σ_{123} (15). In the special situation where all the entries of the density matrix σ_{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

There are severe constraints on how the quantum correlations are distributed among the different parts of a multipartite system. The distribution of quantum correlations among the subsystems of a multipartite quantum system is constrained by the so-called monogamy relation. 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 [45]. In particular, the geometric discord was proven to follow the monogamy property on all pure three qubits. Here, we shall investigate the distribution among the three qubits in the mixed states of typeρ_{123} (3) and σ_{123} (14).

4.1 Monogamy conditions

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

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

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

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

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

where

$$q_1 = 4(|\ \rho_{14} + \rho_{58}\ | + |\ \rho_{23} + \rho_{67}\ |)^2$$

$$q_2 = 4(|\ \rho_{14} + \rho_{58}\ | - |\ \rho_{23} + \rho_{67}\ |)^2$$

$$q_3 = 2[(\rho_{11} + \rho_{55} - \rho_{33} - \rho_{77})^2 + (\rho_{22} + \rho_{66} - \rho_{44} - \rho_{88})^2]. \tag{78}$$

The state ρ_{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

$$p_1 = p_2 = 0$$

$$p_3 = 2[(\rho_{11} + \rho_{22} - \rho_{33} - \rho_{44})^2 + (\rho_{55} + \rho_{66} - \rho_{77} - \rho_{88})^2]$$

which implies that the geometric discord is indeed zero:

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

It follows that the geometric discord in the three qubit states ρ_{123} (3) is monogamous when

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

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

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

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

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

The two qubit density matrices σ_{12} and σ_{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 σ_{12}, the geometric quantum discord is

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

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 σ_{13}, one gets

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

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 satisfy the monogamy properly when the entries of the density matrix σ_{123} satisfy the inequality

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

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

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

where the pure GHZ-state is given by $|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$. The states ρ_{GHZ} belong to the class of mixed three-qubit states of type ρ_{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

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

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 $\rho_{\mathrm{GHZ}_{12}}$ and $\rho_{\mathrm{GHZ}_{23}}$ respectively. Using the results (77) and (79), one obtains

$$D_g(\rho_{\mathrm{GHZ}_{12}}) = 0 \qquad D_g(\rho_{\mathrm{GHZ}_{13}}) = 0.$$

Using the result (87), one has

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

reflecting that the quantum discord in the states ρ_{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 σ_{123} (14). They are given by

$$\sigma_{\mathrm{W}} = \frac{p}{8}\,\mathbb{I} + (1-p)\,|\mathrm{W}\rangle\langle\mathrm{W}|. \tag{89}$$

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

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

and the geometric discord reads as

$$D_{\mathrm{g}}(\sigma_{\mathrm{W}}) = \frac{4}{9}(1-p)^2. \tag{90}$$

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

$$D_{\mathrm{g}}(\sigma_{\mathrm{W}_{12}}) = D_{\mathrm{g}}(\sigma_{\mathrm{W}_{13}}) = \frac{1}{6}(1-p)^2. \tag{91}$$

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

$$D_g(\rho_{\mathrm{W}}) \geq D_g(\rho_{\mathrm{W}_{12}}) + D_g(\rho_{\mathrm{W}_{13}}). \tag{92}$$

The geometric measure of quantum discord in the states σ_{W} satisfies the monogamy condition.

4.2.3 Three-qubit state of Bell type

Finally, we consider the three-qubit

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

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

$$\rho_{\mathrm{B}} = \frac{1}{8}\begin{pmatrix} 1+c_3 & 0 & 0 & 0 & 0 & 0 & 0 & c_1+ic_2 \\ 0 & 1-c_3 & 0 & 0 & 0 & 0 & c_1-ic_2 & 0 \\ 0 & 0 & 1-c_3 & 0 & 0 & c_1-ic_2 & 0 & 0 \\ 0 & 0 & 0 & 1+c_3 & c_1+ic_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_1-ic_2 & 1-c_3 & 0 & 0 & 0 \\ 0 & 0 & c_1+ic_2 & 0 & 0 & 1+c_3 & 0 & 0 \\ 0 & c_1+ic_2 & 0 & 0 & 0 & 0 & 1+c_3 & 0 \\ c_1-ic_2 & 0 & 0 & 0 & 0 & 0 & 0 & 1+c_3 \end{pmatrix}. \tag{94}$$

From equations (63), one has

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

and the geometric discord in the bipartition $1|23$ is

$$D_{\mathrm{g}}(\rho_B) = \frac{1}{8}(c_1^2 + c_2^2 + c_3^2 - c^2) \tag{95}$$

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.*, $D_{\mathrm{g}}(\rho_{B_{12}}) = D_{\mathrm{g}}(\rho_{B_{13}}) = 0$). The quantum $D_{\mathrm{g}}(\rho_B)$ is always non negative and therefore the geometric discord in the states ρ_{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 worth to notice that the geometric measure of quantum discord obtained in this paper are useful for many purposes. First, it provides the explicit amount of quantum correlation in mixed three qubit X states that is generalizable to arbitrary quantum systems of arbitrary number of qubits. Also, it offers a computable tool to get the multipartite quantum correlation defined as the sum of all pairwise partition in a multi-components system (see for instance [44]). In this sense, the present approach constitutes a good alternative to evaluate tripartite correlation in mixed states generalizing the analysis done for pure tripartite systems [45, 44, 46]. In other hand, this approach is ready to adapt in investigating the dynamics of geometric discord in quantum systems subjected to decoherence mechanisms in the spirit of the results recently presented in [47]. Further study in this direction might be worthwhile.

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