Geometric measure of quantum discord and total quantum correlations in an $N$-partite quantum state

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Received 1 May 2012, in final form 28 June 2012
Published 2 August 2012
Online at stacks.iop.org/JPhysA/45/345301

Abstract
Quantum discord, as introduced by Ollivier and Zurek (2001 Phys. Rev. Lett. 88 017901), is a measure of the discrepancy between quantum versions of two classically equivalent expressions for mutual information and is found to be useful in quantification and application of quantum correlations in mixed states. It is viewed as a key resource present in certain quantum communication tasks and quantum computational models without containing much entanglement. An early step toward the quantification of quantum discord in a quantum state was by Dakic et al (2010 Phys. Rev. Lett. 105 190502) who introduced a geometric measure of quantum discord and derived an explicit formula for any two-qubit state. Recently, Luo and Fu (2010 Phys. Rev. A 82 034302) introduced a generic form of the geometric measure of quantum discord for a bipartite quantum state. We extend these results and find generic forms of the geometric measure of quantum discord and total quantum correlations in a general $N$-partite quantum state. Further, we obtain computable exact formulas for the geometric measure of quantum discord and total quantum correlations in an $N$-qubit quantum state. The exact formulas for the $N$-qubit quantum state can be used to get experimental estimates of the quantum discord and the total quantum correlation.

PACS numbers: 03.65.Ud, 75.10.Pq, 05.30.−d

1. Introduction

In quantum information theory, the problem of characterization of correlations present in a quantum state has been a fundamental problem generating intense research effort in the last two decades [1, 2]. Correlations in quantum states, with far-reaching implications for quantum information processing, are usually studied in the entanglement-versus-separability framework [1, 3]. However, some results showed that quantum correlations cannot only be limited to entanglement, because separable quantum states can also have correlations which are
responsible for the improvement of some quantum tasks that cannot be achieved by classical means [4–10]. An alternative classification for correlations based on quantum measurements has arisen in recent years and also plays an important role in quantum information theory [11–14]. This is the quantum-versus-classical paradigm for correlations. The first attempts in this direction were made by Ollivier and Zurek [15] and by Henderson and Vedral [16], who studied quantum correlations from a measurement perspective and introduced quantum discord as a measure of quantum correlations which has generated increasing interest [17–47]. Recently, it was suggested that the quantum discord \( D(\rho) \) can be expressed alternatively as the minimal loss of correlations caused by the non-selective von Neumann projective measurement given by the set of orthogonal 1D projectors \( \{\Pi^a_i\} \) acting on one part of the system [48],

\[
D(\rho) = \min_{\Pi^a} \{ I(\rho) - I(\Pi^a(\rho)) \},
\]

where

\[
\Pi^a(\rho) = \sum_i (\Pi^a_i \otimes I^b)\rho(\Pi^a_i \otimes I^b).
\]

Here the minimum is over the von Neumann measurements \( \Pi^a = \{\Pi^a_i\} \) on a part say \( a \) of a bipartite system \( ab \) in a state \( \rho \) with reduced density operators \( \rho^a \) and \( \rho^b \) and \( \Pi^a(\rho) \) is the resulting state after the measurement. \( I(\rho) = S(\rho^a) + S(\rho^b) - S(\rho) \) is the quantum mutual information, \( S(\rho) = -\text{tr}(\rho \ln \rho) \) is the von Neumann entropy and \( I^b \) is the identity operator on part \( b \).

The definition of quantum discord in terms of quantum mutual information has the disadvantage that it is very difficult to generalize to the multipartite case [49]. We can overcome this hurdle by introducing a geometric measure of quantum discord as the distance of the given state to the closest classical quantum (or the zero discord) state (see equation (6)). Dakic et al [50] introduced a geometric measure of quantum discord given by

\[
D(\rho) = \min_{\chi \in \Omega_0} \|\rho - \chi\|^2,
\]

where \( \Omega_0 \) denotes the set of zero-discord states and \( \|\rho - \chi\|^2 := \text{tr}(\rho - \chi)^2 \) is the square norm in the Hilbert–Schmidt space of linear operators acting on the state space of the system.

Dakic et al [50] also obtained an easily computable exact expression for the geometric measure of quantum discord for a two-qubit system, which can be described as follows. Consider a two-qubit state \( \rho \) expressed in its Bloch representation (see section 3) as

\[
\rho = \frac{1}{4} \left( I^a \otimes I^b + \sum_{a=1}^{3} (x_a \sigma_a \otimes I^b + I^a \otimes y_a \sigma_a) + \sum_{a,b=1}^{3} t_{ab} \sigma_a \otimes \sigma_b \right),
\]

with \( \{\sigma_a\} \) being the Pauli operators. Then its geometric measure of quantum discord is given by [50]

\[
D(\rho) = \frac{1}{4} (||x||^2 + ||T||^2 - \lambda_{\max}).
\]

Here \( \vec{x} := (x_1, x_2, x_3)^t \) and \( \vec{y} := (y_1, y_2, y_3)^t \) are the coherent (column) vectors for single-qubit reduced density operators, \( T = (t_{ab}) \) is the correlation matrix and \( \lambda_{\max} \) is the largest eigenvalue of the matrix \( x\vec{x}^t + TT^t \). The norms of vectors and matrices are the Euclidean norms, for example, \( ||x||^2 := \sum_a x_a^2 \). Here and throughout this paper, the superscript \( t \) denotes the transpose of vectors and matrices and by the norm of any tensor, we mean its Euclidean norm, that is, the square of the norm of a tensor is the sum of squares of its elements.

It is obvious that an exactly computable and experimentally implementable formula for the quantum discord and the total quantum correlations in an \( N \)-partite quantum state is both practically and fundamentally advantageous. It can open up the possibility of
quantitative analysis and experimentation regarding the quantum correlations in a multipartite quantum system. In particular, this can quantitatively determine the evolution of the quantum correlations in a multipartite setting via some quantum information processing protocol.

In this paper,

- we obtain a generic form for the quantum discord $D_k$ (corresponding to the von Neumann measurement on the $k$th part) in an $N$-partite quantum state (section 2, theorem 1);
- we give a formula for the quantum discord $D_k$ in an $N$-qubit quantum state, which is exactly computable as well as experimentally implementable (section 3, theorem 2);
- we apply the exact formula for $D_k$ (obtained in section 3) to some multiqubit states (section 4);
- we give a generic form for the total quantum correlations in a bipartite state which can be exactly computed and experimentally implemented for a two-qubit state (section 5);
- we give a generic form for the total quantum correlations in an $N$-partite state which can be exactly computed and experimentally implemented for an $N$-qubit state (section 6);
- we describe the experimental implementation of the exact formulas for the quantum discord and total quantum correlation in an N-qubit case and also discuss the experimental and computational complexities of these formulas (section 7).

Finally, we summarize in section 8.

2. Quantum discord in an $N$-partite state

Consider a multipartite system $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N$ with $\dim(\mathcal{H}^m) = d_m$, $m = 1, 2, \ldots, N$. Let $L(\mathcal{H}^m)$ be the Hilbert–Schmidt space of linear operators on $\mathcal{H}^m$ with the Hilbert–Schmidt inner product

$$\langle X^{(m)}, Y^{(m)} \rangle := \text{tr} X^{(m)} Y^{(m)}.$$

We can define the Hilbert–Schmidt space $L(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N)$ similarly. Let $\{X_i^{(m)} : i = 1, 2, \ldots, d^2_m, m = 1, 2, \ldots, N\}$ be a set of Hermitian operators which constitute orthonormal bases for $L(\mathcal{H}^m)$; then

$$\text{tr} X_i^{(m)} X_j^{(m)} = \delta_{ij},$$

and $\{X_i^{(1)} \otimes X_i^{(2)} \otimes \cdots \otimes X_i^{(N)}\}$ constitutes an orthonormal basis for $L(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N)$. In particular, any $N$-partite state $\rho_{12\ldots N} \in L(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N)$ can be expanded as

$$\rho_{12\ldots N} = \sum_{i_1i_2\ldots i_N} c_{i_1i_2\ldots i_N} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_N}^{(N)}, \quad i_m = 1, \ldots, d^2_m; \quad m = 1, \ldots, N,$$  \hspace{1cm} (4)

with $C = [c_{i_1i_2\ldots i_N}] = [\text{tr}(\rho_{12\ldots N} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_N}^{(N)})]$ an $N$-way array (tensor of order $N$) with size $d^2_1 d^2_2 \cdots d^2_N$.

We can define the geometric measure of quantum discord for an $N$-partite quantum state corresponding to the von Neumann measurement on the $k$th part as

$$D_k(\rho_{12\ldots N}) = \min_{\chi_k} \|\rho_{12\ldots N} - \chi_k\|^2,$$  \hspace{1cm} (5)

where the minimum is over the set of zero discord states $\chi_k$ (i.e. $D_k(\chi_k) = 0$) [51]. A state $\chi_k \in L(\mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N)$ is of zero discord if and only if it is a classical-quantum state [52].

$$\chi_k = \sum_{l=1}^{d_k} p_l |l\rangle \langle l| \otimes \rho_{(k)l},$$  \hspace{1cm} (6)
where \(|k\rangle\) stands for \(12\cdots(k - 1)(k + 1)\cdots N\). \(|p_i\rangle\) is a probability distribution over the terms in the sum, \(|\langle l\rangle|\) is an arbitrary orthonormal basis in \(H^k\) and \([\rho_{[kl]}]\) is a set of arbitrary states (density operators acting on \(H^1 \otimes H^2 \otimes \cdots \otimes H^{k-1} \otimes H^{k+1} \otimes \cdots \otimes H^d\)). It follows that the quantum discord corresponding to the measurement on different subsystems is different, that is, \(D_k(\rho) \neq D_l(\rho)\), \(k \neq l\).

We need to define a product of a tensor with a matrix, the \(n\)-mode product [53, 54]. The \(n\)-mode (matrix) product of a tensor \(\mathcal{Y}\) of order \(N\) and with dimension \(J_1 \times J_2 \times \cdots \times J_N\) with a matrix \(A\) with dimension \(I \times J_0\) is denoted by \(\mathcal{Y} \times_n A\). The result is a tensor of size \(J_1 \times J_2 \times \cdots \times J_{n-1} \times I\) and \(n\)-mode product is given in [48] and leads to its natural generalization.

**Theorem 1.** Let \(\rho_{12\cdots N}\) be an \(N\)-partite state defined by equation (4); then

\[
D_k(\rho_{12\cdots N}) = \|C\|^2 - \max_{A(k)} \|C \times_k A(k)\|^2, \tag{9}
\]

where \(C = [c_{ij}]\) is a \(d_k^2 \times d_k^2\) matrix and the maximum is taken over all \(d_k \times d_k^2\)-dimensional isometric matrices \(A(k) = [a_{ik}], \quad A(k)'(A(k)^{t})' = I_k\), such that \(a_{ik} = \text{tr}(\langle l \rangle|\langle l|^1 \rangle^t X_{ik}^{(k)}), \quad l = 1, 2, \ldots, d_k, \quad a_{ik} = \text{tr}(\langle l \rangle|\langle l|^1 \rangle^t X_{ik}^{(k)}), \quad l = 1, 2, \ldots, d_k, \quad [\langle l\rangle]\) is any orthonormal basis in \(H^k\). We generalize this result to \(N\)-partite quantum states. The proof of theorem 1 below runs on similar lines as that of equation (8) given in [48] and leads to its generalization.

**Proof.** We expand the operator \(|l\rangle\langle l|\) occurring in the expression for the zero discord state \(\chi_k\) (equation (6)) in the orthonormal basis \(\{X_{ik}^{(k)}\}\) in \(L(H^k)\) as

\[
|l\rangle\langle l| = \sum_{i_k=1}^{d_k^2} a_{ik} X_{ik}^{(k)}, \quad l = 1, 2, \ldots, d_k; \tag{10}
\]

with

\[
a_{ik} = \text{tr}(\langle l\rangle\langle l|X_{ik}^{(k)}\rangle) = \langle l|X_{ik}^{(k)}|l\rangle, \tag{11}
\]

\(|\langle l|\rangle\) being any orthonormal basis in \(H^k\). Clearly, \(\sum_{l=1}^{d_k} a_{il} = \text{tr} X_{il}^{(k)}\). Arranging the coefficients in a row vector as

\[
\vec{a}_{i} = (a_{i1}, a_{i2}, \ldots, a_{id_k}),
\]

we obtain, by the Parseval theorem of abstract Fourier transform,

\[
||\vec{a}_{i}||^2 = |||\langle l\rangle\langle l|\rangle||^2 = 1. \tag{12}
\]

Here ||\vec{a}_{i}||^2 = \(\sum a_{il}^2\). Moreover, the orthonormality of \(|\langle l\rangle\rangle\) implies that \(\vec{a}_{i}\) is an orthonormal set of vectors, and therefore \(A^{(k)} = [a_{il}]\) is an isometry in the sense that \(A^{(k)}(A^{(k)})' = I_k\).
Similarly, because \( \{X_{t_1}^{(1)} \otimes X_{t_2}^{(2)} \otimes \cdots \otimes X_{t_{k-1}}^{(k-1)} \otimes X_{t_k}^{(k+1)} \otimes \cdots \otimes X_{t_N}^{(N)} \} \) constitutes an orthonormal basis for \( \mathcal{H} \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_m \otimes \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N \), we can expand the operator \( \rho_{[k][l]} \) occurring in the expression for the zero discord state \( \rho_k \) as

\[
p_{l}[\rho_{[k][l]}] = \sum_{i_1,i_2,\ldots,i_{k-1},i_{k+1},\ldots,i_N} b_{i_1i_2\cdots i_{k-1}i_{k+1}\cdots i_N} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_{k-1}}^{(k-1)} \otimes X_{i_{k+1}}^{(k+1)} \otimes \cdots \otimes X_{i_N}^{(N)},
\]

where the maximum is taken over \( l \), \( m = 1, 2, \ldots, d_m^2 \); \( m = 1, \ldots, k - 1, k + 1, \ldots, N \), with \( b_{i_1i_2\cdots i_{k-1}i_{k+1}\cdots i_N} = \text{tr}(\rho_{[k][l]} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_{k-1}}^{(k-1)} \otimes X_{i_{k+1}}^{(k+1)} \otimes \cdots \otimes X_{i_N}^{(N)}) \). Then we have, using the orthonormality of the \( X \) basis,

\[
\sum_{i_1,i_2,\ldots,i_{k-1},i_{k+1},\ldots,i_N} b_{i_1i_2\cdots i_{k-1}i_{k+1}\cdots i_N}^2 = \rho_k^2 \text{tr} \rho_{[k][l]}^2. \tag{13}
\]

In view of equations (5) and (6), the square norm distance between \( \rho_{12} - \chi_k \) can be evaluated (using the orthonormality of the bases involved and equation (13)) as

\[
||\rho_{12} - \chi_k||^2 = \text{tr} \rho_{12}^2 - 2\text{tr}(\rho_{12} - \chi_k) + \text{tr} \chi_k^2
\]

\[
= \sum_{i_1,i_2,\ldots,i_N} c_{i_1i_2\cdots i_N}^2 - 2 \sum_{i_1,i_2,\ldots,i_N} c_{i_1i_2\cdots i_N} \sum_l p_{l}[l] X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_{k-1}}^{(k-1)} \otimes X_{i_{k+1}}^{(k+1)} \otimes \cdots \otimes X_{i_N}^{(N)} + \sum_l \rho_k^2 \text{tr} \rho_{[k][l]}^2
\]

\[
= ||C||^2 - 2 \sum_{i_1,i_2,\ldots,i_N} c_{i_1i_2\cdots i_N} \sum_l d_{l} a_{l} b_{i_1i_2\cdots i_{k-1}i_{k+1}\cdots i_N} + \sum_{i_1,i_2,\ldots,i_N} b_{i_1i_2\cdots i_{k-1}i_{k+1}\cdots i_N}^2
\]

\[
= ||C||^2 - \sum_{i_1,i_2,\ldots,i_N} \left( \sum_l c_{i_1i_2\cdots i_N} a_{l} \right)^2 + \sum_{i_1,i_2,\ldots,i_N} \left( b_{i_1i_2\cdots i_{k-1}i_{k+1}\cdots i_N} - \sum_l c_{i_1i_2\cdots i_N} a_{l} \right)^2. \tag{14}
\]

By choosing \( b_{i_1i_2\cdots i_{k-1}i_{k+1}\cdots i_N} = \sum_l c_{i_1i_2\cdots i_N} a_{l} \), the above equation reduces to

\[
||\rho_{12} - \chi_k||^2 = ||C||^2 - ||C \times A^{(k)}||^2.
\]

Since the tensor \( C \) is determined by the state \( \rho_{12} \) via equation (4), we have, using equation (2),

\[
D_k(\rho_{12}) = \min_{\Delta_k} ||\rho_{12} - \chi_k||^2 = ||C||^2 - \max_{A^{(k)}} ||C \times A^{(k)}||^2,
\]

where the maximum is taken over \( A^{(k)} \) specified in the theorem, thus completing the proof. \( \Box \)

For a bipartite system, \( C \) is a \( d_1^2 \times d_2^2 \) matrix, while \( A^{(1)} \) and \( A^{(2)} \) are the \( d_1 \times d_1^2 \) and \( d_2 \times d_2^2 \) matrices, respectively. Using the definition of the \( n \)-mode product (equation (7)) and the norm of a tensor, it follows that

\[
D_k(\rho) = \text{tr}(CC^c) - \max_{A^{(1)}} \text{tr}(A^{(1)}CC^cA^{(1)c}), \tag{15}
\]

which amounts to choosing for \( \sum_l p_{l} \rho_{[l]} \) the reduced density operator obtained by tracing out the \( k \)th part from the state \( \rho_{12} \) (equation (4)), which can always be done because \( \{\rho_{[k][l]}\} \) is a set of arbitrary density operators acting on \( \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_m \otimes \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_N \) and \( \{p_l\} \) is an arbitrary probability distribution.
and

\[ D_2(\rho) = \text{tr}(CC^*) - \max_{A(\rho)} \text{tr}(A^{(1)}C^*A^{(2)}) \]  

(16)

Following its definition in equation (1), it seems more natural and simple to define the geometric measure of quantum discord as

\[ \overline{D}_k(\rho_{12\ldots N}) = \min_{\Pi^k} \|\rho_{12\ldots N} - \Pi^k(\rho_{12\ldots N})\|^2, \]  

(17)

where the minimum is over the von Neumann measurements \( \Pi^k = \{\Pi_i^k\} \) on the system \( \mathcal{H}^k \), and \( \Pi^k(\rho_{12\ldots N}) = \sum_i (I_1 \otimes I_2 \otimes \cdots \otimes I_i^k \otimes \cdots \otimes I_N) \rho_{12\ldots N} (I_1 \otimes I_2 \otimes \cdots \otimes I_i^k \otimes \cdots \otimes I_N) \).

It is easy to prove that \( D_k(\rho_{12\ldots N}) = \overline{D}_k(\rho_{12\ldots N}) \), similar to theorem 2 in [48].

3. Exact formula for an \( N \)-qubit state

In this section, we specialize to the \( N \)-qubit systems with states in \( \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2 \) \((N \text{ factors})\). We need the structure of the Bloch representation of density operators, which can be briefly described as follows. The Bloch representation of a density operator acting on the Hilbert space of a \( d \)-level quantum system \( \mathbb{C}^d \) is given by

\[ \rho = \frac{1}{d} \left( I_d + \sum_a s_a \lambda_a \right), \]  

(18)

where the components of the coherent vector \( \vec{s} \), defined via equation (18), are given by \( s_a = \frac{i}{d} \text{tr}(\rho \lambda_a) \). Equation (18) is the expansion of \( \rho \) in the Hilbert–Schmidt basis \( \{I, \lambda_a; \alpha = 1, 2, \ldots, d^2 - 1\} \) where \( \lambda_a \) are the traceless Hermitian generators of \( SU(d) \) satisfying \( \text{tr}(\lambda_a \lambda_b) = 2\delta_{ab} \) [55].

In order to give the Bloch representation of a density operator acting on the Hilbert space \( \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2 \) of an \( N \)-qubit quantum system, we introduce the following notation. We use \( k_i \) \((i = 1, 2, \ldots)\) to denote a qubit chosen from \( N \) qubits, so that \( k_i \) \((i = 1, 2, \ldots)\) take values in the set \( \mathcal{N} = \{1, 2, \ldots, N\} \). Thus, each \( k_i \) is a variable taking values in \( \mathcal{N} \). The variables \( k_1 = 1, 2, 3 \) for a given \( k_i \) span the set of generators of the \( SU(2) \) group (except identity) for the \( k_i\)th qubit, namely the set of Pauli operators \( \{\sigma_1, \sigma_2, \sigma_3\} \) for the \( k_i\)th qubit. For two qubits \( k_1 \) and \( k_2 \), we define

\[ \sigma_{a_{k_1}} = (I_2 \otimes I_2 \otimes \cdots \otimes \sigma_{a_{k_1}} \otimes I_2 \otimes \cdots \otimes I_2) \]

\[ \sigma_{a_{k_2}} = (I_2 \otimes I_2 \otimes \cdots \otimes \sigma_{a_{k_2}} \otimes I_2 \otimes \cdots \otimes I_2) \]

\[ \sigma_{a_{k_1}} \sigma_{a_{k_2}} = (I_2 \otimes I_2 \otimes \cdots \otimes \sigma_{a_{k_1}} \otimes I_2 \otimes \cdots \otimes \sigma_{a_{k_2}} \otimes I_2 \otimes I_2), \]  

(19)

where \( \sigma_{a_{k_1}} \) and \( \sigma_{a_{k_2}} \) occur at the \( k_1\)th and \( k_2\)th places (corresponding to the \( k_1\)th and \( k_2\)th qubits, respectively) in the tensor product and are the \( a_{k_1}\)th and \( a_{k_2}\)th generators of \( SU(2) \), \( a_{k_1} = 1, 2, 3 \) and \( a_{k_2} = 1, 2, 3 \), respectively. Then we can write, for an \( N \)-qubit state \( \rho_{12\ldots N} \),

\[ \rho_{12\ldots N} = \frac{1}{2^N} \left\{ \bigotimes_{k \in \mathcal{N}} I_2 + \sum_{k_1 \in \mathcal{N}} \sum_{a_{k_1}} s_{a_{k_1}} \sigma_{a_{k_1}}^{(1)} + \sum_{[k_1,k_2]} \sum_{a_{k_1}a_{k_2}} t_{a_{k_1}a_{k_2}} \sigma_{a_{k_1}}^{(1)} \sigma_{a_{k_2}}^{(2)} + \cdots \right. \]

\[ + \left. \sum_{[k_1,k_2,\ldots,k_M]} \sum_{a_{k_1}a_{k_2}\ldots a_{k_M}} t_{a_{k_1}a_{k_2}\ldots a_{k_M}} \sigma_{a_{k_1}}^{(1)} \sigma_{a_{k_2}}^{(2)} \cdots \sigma_{a_{k_M}}^{(N)} \right\}, \]  

(20)
where \( s^{(k)} \) is a Bloch (coherent) vector corresponding to the \( k \)th qubit, \( s^{(k)} = \left[ \alpha_{ki} \right]_{\alpha_i = 1}^3 \), which is a tensor of order 1 defined by

\[
\sigma_{\alpha_i \sigma} = \text{tr} \left[ \rho \sigma_{\alpha_i} \right] = \text{tr} \left[ \rho_k \sigma_{\alpha_i} \right],
\]

(21)

where \( \rho_k \) is the reduced density matrix for the \( k \)th qubit. Here \( \{k_1, k_2, \ldots, k_M\} \) is a subset of \( \mathcal{N} \) and can be chosen in \( \binom{\mathcal{N}}{M} \) ways, contributing the \( \binom{\mathcal{N}}{M} \) terms in the sum \( \sum_{k_1, k_2, \ldots, k_M} \) in equation (20), each containing a tensor of order \( M \). The total number of terms in the Bloch representation of \( \rho \) is \( 2^N \). We denote the tensors occurring in the sum \( \sum_{k_1, k_2, \ldots, k_M} \) (2 \( \leq M \leq \mathcal{N} \)) by \( T^{[k_1, k_2, \ldots, k_M]} = \left[ t_{\alpha_{k_1} \alpha_{k_2} \ldots \alpha_{k_M}} \right] \) which are defined by

\[
t_{\alpha_{k_1} \alpha_{k_2} \ldots \alpha_{k_M}} = \text{tr} \left[ \rho_{k_1, k_2, \ldots, k_M} \right] \left( \sigma_{\alpha_{k_1}} \otimes \sigma_{\alpha_{k_2}} \otimes \ldots \otimes \sigma_{\alpha_{k_M}} \right),
\]

(22)

where \( \rho_{k_1, k_2, \ldots, k_M} \) is the reduced density matrix for the subsystem \( \{k_1, k_2, \ldots, k_M\} \). We call the tensor in the last term in equation (20) \( T^{(N)} \).

In this paper, we find the maximum in equation (9) for an \( N \)-qubit state \( \rho_{12, \ldots, N} \) to obtain an exact analytic formula, as in the two-qubit case (equation (3)) [50].

**Theorem 2.** Let \( \rho_{12, \ldots, N} \) be an \( N \)-qubit state defined by equation (20); then

\[
D_k(\rho_{12, \ldots, N}) = \frac{1}{2N} \left[ ||s^{(k)}||^2 + \sum_{1 \leq M \leq \mathcal{N} - 1} \sum_{\{k_1, \ldots, k_M\} \subseteq \mathcal{N} - \{k\}} ||T^{[k_1, \ldots, k_M]}||^2 \right] - \eta_{\text{max}},
\]

(23)

Here \( \eta_{\text{max}} \) is the largest eigenvalue of the matrix \( G^{(k)} \) which is a \( 3 \times 3 \) real symmetric matrix, defined as

\[
G^{(k)} = s^{(k)} (s^{(k)})^T + \sum_{k \in \mathcal{N} - \{k\}} (T^{[k, \ldots, k]} (T^{[k, \ldots, k]})^T + \sum_{2 \leq M \leq \mathcal{N} - 1} T^{(M + 1)}),
\]

(24)

where \( T^{(M + 1)} = \left[ t^{(M + 1)} \right] \) are the \( 3 \times 3 \) matrices, defined elementwise as

\[
t_{\alpha_{k_1} \alpha_{k_2} \ldots \alpha_{k_{M + 1}}} = \sum_{\{k_1, \ldots, k_M\} \subseteq \mathcal{N} - \{k\}} \sum_{\alpha_{k_{M + 1}}} t_{\alpha_{k_1} \alpha_{k_2} \ldots \alpha_{k_{M + 1}}} \delta_{\alpha_{k_1} \alpha_{k_2} \ldots \alpha_{k_{M + 1}}},
\]

\[
\alpha_{k_1}, \alpha_{k_2}, \beta_k = 1, 2, 3; \ i = 1, 2, \ldots, M.
\]

**Proof.** Our goal is to obtain a closed form expression for the term \( \max_{A^{(k)}} ||C \times A^{(k)}||^2 \) in equation (9) applied to an arbitrary state \( \rho_{12, \ldots, N} \) of an \( N \)-qubit system. The tensor \( C = \left[ c_{i_1 i_2 \ldots i_N} \right] \) determined by the \( N \)-qubit state \( \rho_{12, \ldots, N} \) via equation (4) has \( i_m = 1, 2, 3, 4; m = 1, 2, \ldots, N \), having \( 4^N \) elements in it. The \( 2 \times 4 \) isometric matrices \( A = \left[ a_{i_k} \right] \) have to satisfy \( a_{i_k} = \text{tr} ||(i_{X_i^{(k)}}) || \). In other words, the row vectors of \( A^{(k)} \) must satisfy equation (18) for some single-qubit pure state. However, it is well known that every unit vector \( \hat{s} \) in \( \mathbb{R}^3 \) (which corresponds to a point on the Bloch sphere) satisfies equation (18) for some single-qubit pure state (which is not true for a higher dimensional system [56, 57]). Therefore, we can obtain the required maximum over isometric \( 2 \times 4 \) matrices in the form obtained below (see equations (31) and (32)).

We choose the orthonormal bases \( \left\{ X^{(m)}_{i_m} \right\} \), \( i_m = 1, 2, 3, 4; \ m = 1, 2, \ldots, N \), in equation (4) as the generators of \( SU(2_{m}) \), \( m = 1, 2, \ldots, N \) [48],

\[
X^{(m)}_{i_m} = \frac{1}{\sqrt{2}} \sigma_{i_{m-1}}, \quad i_m = 1, 2, 3, 4; \quad m = 1, 2, \ldots, N,
\]

(25)

and

\[
X^{(m)}_{i_m} = \frac{1}{\sqrt{2}} \sigma_{i_{m-1}}, \quad i_m = 1, 2, 3, 4; \quad m = 1, 2, \ldots, N,
\]

(26)

where \( \sigma_{1,2,3} \) stand for the Pauli operators acting on the \( m \)th qubit.
Since $\text{tr} \sigma_{ai} = 0$, $\alpha_k = 1, 2, 3$, we have
\[
\sum_{l=1}^{2} a_{li} = \text{tr} \chi^{(k)}_{li} = \frac{1}{\sqrt{2}} \text{tr} \sigma_{ai-1} = 0, \quad i_k = 2, 3, 4.
\]
Therefore,
\[
a_{2i} = -a_{1i}, \quad i_k = 2, 3, 4. \quad (27)
\]
We now proceed to construct the $2 \times 4$ matrix $A^{(k)}$ defined via equation (11). We will use equation (27). The row vectors of $A^{(k)}$ are
\[
\tilde{a}_i = (a_{1i}, a_{2i}, a_{3i}, a_{4i}), \quad i = 1, 2.
\]
Next we define
\[
\hat{e}_i = \sqrt{2} (a_{1i}, a_{2i}, a_{3i}, a_{4i}), \quad i = 1, 2,
\]
and using equation (27), we obtain
\[
\hat{e}_2 = -\hat{e}_1. \quad (29)
\]
We can prove
\[
||\hat{e}_i||^2 = 1, \quad i = 1, 2, \quad (30)
\]
using the condition $||\tilde{a}_i||^2 = \sum_{k=1}^{4} a_{ki}^2 = 1$ (equation (12)) and using $a_{1i} = \text{tr}(|l|/\ell|\chi^{(k)}_{1i}|) = \frac{1}{\sqrt{2}}$.

We can now construct the row vectors of the $2 \times 4$ matrix $A^{(k)}$, using equations (28) and (29):
\[
\tilde{a}_1 = \frac{1}{\sqrt{2}} (1, \hat{e}_1), \quad (31)
\]
\[
\tilde{a}_2 = \frac{1}{\sqrt{2}} (1, -\hat{e}_1). \quad (32)
\]

The matrix $A^{(k)}$ is, in terms of its row vectors defined above,
\[
A^{(k)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \hat{e}_1 \\ 1 & -\hat{e}_1 \end{pmatrix}.
\]

The norm of the tensor $C$ can be expressed in terms of the norms of the tensors defining $\rho_{1 \cdots N}$ by using the equivalence of the definitions of $\rho_{1 \cdots N}$ given in equations (4) and (20) as
\[
||C||^2 = \frac{1}{2N} \left[ 1 + \sum_{k_i \in N} ||\sigma^{(k_i)}||^2 + \sum_{[k_1, k_2]} ||T^{(k_1, k_2)}||^2 + \ldots \right.
\]
\[
\left. + \sum_{[k_1, k_2, \ldots, k_d]} ||T^{(k_1, k_2, \ldots, k_d)}||^2 + \ldots + ||T^{(N)}||^2 \right]. \quad (33)
\]

In order to obtain the norm of $C \times_k A^{(k)}$, we use its elementwise definition,
\[
(C \times_k A^{(k)})_{i_1i_2 \cdots i_d i_{d+1} \cdots i_N} = \sum_{a_i} c_{i_1i_2 \cdots i_d} a_{i_{d+1} i_{d+2} \cdots i_N} a_{i_{d+3} \cdots i_N}, \quad i = 1, 2, \quad (34)
\]
the equivalence of the definitions of $\rho_{1 \cdots N}$ given in equations (4) and (20) and the elements of $A^{(k)}$ given by equations (31) and (32). The result is
\[
||C \times_k A^{(k)}||^2 = \frac{1}{2N} \left[ 1 + \sum_{k_i \in N \setminus \{k\}} ||\sigma^{(k_i)}||^2 + \sum_{2 \leq M \leq N-1} \sum_{[k_1, k_2, \ldots, k_M]} ||T^{(k_1, k_2, \ldots, k_M)}||^2 \right.
\]
\[
\left. + \hat{e}_1 \sigma^{(k)} (\sigma^{(k)})' \hat{e}_1' + \sum_{k_i \in N \setminus \{k\}} \hat{e}_1 (T^{(k_1, k_i)})' T^{(k_1, k_i)} \hat{e}_1' \right.
\]
\[
\left. + \sum_{2 \leq M \leq N-1} \sum_{[k_1, k_2, \ldots, k_M \in N \setminus \{k\}]} \sum_{a_{i_1} \cdots a_{i_M}} (\hat{e}_1)_{a_{i_1} a_{i_2} a_{i_3}} (\sum_{a_{i_4} \cdots a_{i_M}} (\hat{e}_1)_{a_{i_4}} (a_{i_1} a_{i_2} a_{i_3} a_{i_4})) (\hat{e}_1)_{a_{i_4}} \right]. \quad (35)
\]
or
\[ ||C \times k A^{(k)}||^2 = \frac{1}{2N} \left( 1 + \sum_{k_i \in N^{\prime} - \{\bar{k}\}} ||x^{(k_i)}||^2 + \sum_{2 \leq M \leq N-1} \sum_{\{k_1, k_2, \ldots, k_M\} \subseteq N^{\prime} - \{\bar{k}\}} ||T^{\{k_1, k_2, \ldots, k_M\}}||^2 \right) \]
\[ + \hat{\epsilon}_1 \left[ \tilde{s}^{(k)} (\tilde{s}^{(k)})^T + \sum_{k_i \in N^{\prime} - \{\bar{k}\}} (T^{\{k_1, k_i\}})^T T^{\{k_1, k_i\}} + \sum_{2 \leq M \leq N-1} \tau^{(M+1)} \right] \eta_1^2 \right], \quad (36) \]

where \( \tau^{(M+1)} = [\tau_{ab, \beta_k}^{(M+1)}] \) with
\[ \tau_{ab, \beta_k}^{(M+1)} = \sum_{\beta_1, \ldots, \beta_k} \sum_{\{a_1, a_2, \ldots, a_k\} \subseteq N^{\prime} - \{\bar{k}\}} f_{a_1, a_2} \cdots f_{a_k, a_{\beta_k}} \alpha_{a_1, a_2, \ldots, a_{\beta_k}}, \]
as in the statement of the theorem.

Let us put the expression in square bracket, the \((3 \times 3)\) real symmetric matrix in equation (36), as
\[ G^{(k)} = \tilde{s}^{(k)} (\tilde{s}^{(k)})^T + \sum_{k_i \in N^{\prime} - \{\bar{k}\}} (T^{\{k_1, k_i\}})^T T^{\{k_1, k_i\}} + \sum_{2 \leq M \leq N-1} \tau^{(M+1)}. \]

Thus, we obtain
\[ ||C \times k A^{(k)}||^2 = \frac{1}{2N} \left( 1 + \sum_{k_i \in N^{\prime} - \{\bar{k}\}} ||x^{(k_i)}||^2 \right) \]
\[ + \sum_{2 \leq M \leq N-1} \sum_{\{k_1, k_2, \ldots, k_M\} \subseteq N^{\prime} - \{\bar{k}\}} ||T^{\{k_1, k_2, \ldots, k_M\}}||^2 + \hat{\epsilon}_1 \eta_1^2. \quad (37) \]

In equation (37), only the last term depends on the matrix \( A^{(k)} \), while all others are determined by the state \( \rho_{1 \cdots N} \). Therefore, to maximize \( ||C \times k A^{(k)}||^2 \), we take \( \hat{\epsilon}_1 \) to be the eigenvector of \( G^{(k)} \) corresponding to its largest eigenvalue \( \eta_{\text{max}} \), so that
\[ \max_{A^{(k)}} ||C \times k A^{(k)}||^2 = \frac{1}{2N} \left( 1 + \sum_{k_i \in N^{\prime} - \{\bar{k}\}} ||x^{(k_i)}||^2 \right) \]
\[ + \sum_{2 \leq M \leq N-1} \sum_{\{k_1, k_2, \ldots, k_M\} \subseteq N^{\prime} - \{\bar{k}\}} ||T^{\{k_1, k_2, \ldots, k_M\}}||^2 + \eta_{\text{max}} \right]. \quad (38) \]

Finally, equations (33), (38) and (9) together imply
\[ D_k(\rho_{1 \cdots N}) = \frac{1}{2N} \left( ||\tilde{s}^{(k)}||^2 + \sum_{1 \leq M \leq N-1} \sum_{\{k_1, k_2, \ldots, k_M\} \subseteq N^{\prime} - \{\bar{k}\}} ||T^{\{k_1, k_2, \ldots, k_M\}}||^2 - \eta_{\text{max}} \right), \]
where \( \eta_{\text{max}} \) is the largest eigenvalue of matrix \( G^{(k)} \), thus completing the proof. \( \square \)

From equations (37) and (38), we note that the isometric \( 2 \times 4 \) matrix \( \tilde{A}^{(k)} \) which maximizes \( ||C \times k A^{(k)}||^2 \) can now be explicitly constructed as
\[ \tilde{A}^{(k)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \hat{\epsilon}_{\text{max}} \\ 1 & -\hat{\epsilon}_{\text{max}} \end{pmatrix}, \]
where \( \hat{\epsilon}_{\text{max}} \) is the eigenvector of \( G^{(k)} \) for its highest eigenvalue \( \eta_{\text{max}} \). We can then use equation (9) directly to compute
\[ D_k(\rho_{1 \cdots N}) = ||C||^2 - ||C \times k \tilde{A}^{(k)}||^2. \quad (39) \]
For a two-qubit system, equation (23) reduces to
\[ D_1(\rho_{12}) = \frac{1}{4}(||\vec{x}||^2 + ||T||^2 - \eta_{\text{max}}). \]  
(40)
and
\[ D_2(\rho_{12}) = \frac{1}{4}(||\vec{y}||^2 + ||T||^2 - \xi_{\text{max}}), \]  
(41)
where \( \vec{x} \) and \( \vec{y} \) are the coherent vectors of the reduced density operators of the first and the second qubit, respectively, \( T \) is the two-qubit correlation matrix, and \( \eta_{\text{max}} \) and \( \xi_{\text{max}} \) are the largest eigenvalues of \( G^{(1)} = \vec{x}\vec{x}^T + TT^t \) and \( G^{(2)} = \vec{y}\vec{y}^T + T^tT \), respectively.

Interestingly, the quantum discord \( D_2(\rho_{12\cdots N}) \) can be obtained experimentally, without any \emph{a priori} knowledge of the state \( \rho_{12\cdots N} \), because all the elements of the matrix \( G^{(2)} \) as well as the tensor \( C \) (equation (4)) (both of which are the average values of the tensor products of Pauli operators in the \( N \)-qubit state) can be experimentally estimated by measuring Pauli operators on individual qubits (see section 7).

4. Examples

Next, we apply our measure to some multiqubit quantum states. Unfortunately, in general, a quantitative comparison with the entanglement-separability scenario still eludes us because a viable measure of entanglement for multipartite mixed states is not available. However, genuine three-qubit entanglement has been studied using the three-tangle [58]. A detailed comparison of this work with the following examples warrants a separate study.

The first example comprises the three-qubit mixed states
\[ \rho = p|\text{GHZ}\rangle\langle\text{GHZ}| + \frac{(1-p)}{8}I_3, \quad 0 \leq p \leq 1; \]  
(42)
where \( |\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle) \) and \( I_3 \) is the identity matrix. Figure 1(a) shows the variation of \( D_1(\rho) \) with \( p \). We see that \( D_1(\rho) \) increases continuously from the \( p = 0 \) state (random mixture) to the \( p = 1 \) state (pure GHZ state), as expected.

The second example is the set of three-qubit states,
\[ \rho = p|W\rangle\langle W| + (1-p)|\text{GHZ}\rangle\langle\text{GHZ}|, \quad 0 \leq p \leq 1; \]  
(43)
where \( |W\rangle = \frac{1}{\sqrt{8}}(|100\rangle + |010\rangle + |001\rangle) \). Figure 1(b) shows the variation of \( D_1(\rho) \) with \( p \). It is straightforward to check that this state cannot be written as a classical quantum state for any value of \( p \), including \( p = \frac{1}{2} \). This explains the nonzero discord at \( p = \frac{1}{2} \). Further, we observe that the discord for the pure GHZ state exceeds that for the pure \( W \) state, in conformity with similar behavior of entanglement in these states [59]. The rate of increase of the discord with \( p \) diminishes discontinuously at \( p = \frac{3}{4} \) as the \( |W\rangle \) state increasingly dominates the classical mixture in equation (43) with increasing \( p \). This interesting observation needs further analysis.

As the last example, we consider the set of three-qubit states,
\[ \rho = p|\text{GHZ}_-\rangle\langle\text{GHZ}_-| + (1-p)|\text{GHZ}\rangle\langle\text{GHZ}|, \quad 0 \leq p \leq 1, \]  
(44)
where \( |\text{GHZ}_-\rangle = \frac{1}{\sqrt{2}}(|000\rangle - |111\rangle) \). Figure 1(c) shows the variation of \( D_1(\rho) \) with \( p \). The discord is symmetric about \( p = \frac{1}{2} \) at which it vanishes. For \( p = \frac{1}{2} \), the state can be written as \( \frac{1}{2}|000\rangle\langle000| + \frac{1}{2}|111\rangle\langle111| \) which is a classical quantum state, so that the discord vanishes at \( p = \frac{1}{2} \). Again, the discord is maximum and equal for the pure \( |\text{GHZ}\rangle \) state and the pure \( |\text{GHZ}_-\rangle \) state, similar to the behavior of entanglement in these two states [59].

We note that, in all these examples, \( D_1(\rho) = D_2(\rho) = D_3(\rho) \) as all the states are symmetric with respect to the swapping of qubits.
Figure 1. Variation of the quantum discord with parameter $p$ for the states given in (a) equations (42), (b) (43) and (c) (44).
5. Total quantum correlations in a bipartite state

Consider a bipartite state \( \rho \) and denote by \( \hat{\Pi}^{(1)} \) the von Neumann measurement minimizing \( \| \rho - \Pi^{(1)}(\rho) \|^{2} \). It is straightforward to check that the state after the measurement \( \hat{\Pi}^{(1)}(\rho) \) is a zero discord state, that is, \( D_{1}(\hat{\Pi}^{(1)}(\rho)) = 0 \). However, the state \( \hat{\Pi}^{(1)}(\rho) \) may have \( D_{2}(\hat{\Pi}^{(1)}(\rho)) \neq 0 \). Thus, the state \( \hat{\Pi}^{(1)}(\rho) \) can have some nonzero quantum correlations. Thus, neither \( D_{1}(\rho) \) nor \( D_{2}(\rho) \) gives us a measure of the total quantum correlations in the state \( \rho \). But this analysis suggests that the quantity

\[
Q(\rho) = D_{1}(\rho) + D_{2}(\hat{\Pi}^{(1)}(\rho))
\]

(45)
gives the required measure of the total quantum correlations in the state \( \rho \) [51].

In order to find the optimal von Neumann measurement \( \hat{\Pi}^{(1)}(\rho) \) on \( \rho \) which minimizes \( \| \rho - \hat{\Pi}^{(1)}(\rho) \|^{2} \), we have to find the corresponding orthonormal basis \( \{|\tilde{q}\rangle \} \) in \( \mathcal{H} \) such that \( \{\hat{\Pi}^{(1)}_{i}\} = \{|\tilde{q}\rangle \langle \tilde{q}|\} \). The expansion of these 1D projectors \( |\tilde{q}\rangle \langle \tilde{q}| \) in the basis \( X_{i} = \{I_{i}, \lambda_{i}\} (\lambda_{i}: \text{generators of } SU(d_{i})) \) via equation (10), that is,

\[
|\tilde{q}\rangle \langle \tilde{q}| = \sum_{i} \tilde{a}_{qi} X_{i}, \quad q = 1, \ldots, d_{1},
\]

(46)
with

\[
\tilde{a}_{qi} = \langle q | X_{i} | \tilde{q} \rangle, \quad q = 1, 2, \ldots, d_{1}; \quad i = 1, \ldots, d_{i}^{2},
\]

(47)
must then give the matrix \( \hat{\Lambda}^{(1)} \) which maximizes \( \text{tr}(AC A') \) which in turn gives \( D_{1}(\rho) \).

To obtain the state \( \hat{\Pi}^{(1)}(\rho) \), we proceed as follows. As noted above, any post-measurement state \( \Pi^{(1)}(\rho) \) is a zero discord state satisfying \( D_{1}(\Pi^{(1)}(\rho)) = 0 \). Hence, \( \Pi^{(1)}(\rho) \) must have the form of the classical quantum state as in equation (6) for \( N = 2 \), namely

\[
\Pi^{(1)}(\rho) = \sum_{q=1}^{d_{1}} p_{q} |q\rangle \langle q| \otimes \rho_{q}.
\]

(48)
We expand the state \( p_{q} \rho_{q} \) in equation (48) in terms of the basis \( \{X_{j}^{(2)}\} \) to obtain

\[
p_{q} \rho_{q} = \sum_{j} b_{qj} X_{j}^{(2)},
\]

(49)
where \( b_{qj} = \text{tr}(p_{q} \rho_{q} X_{j}^{(2)}) \). We know from [48] that, for equation (39) for \( N = 2 \) to hold, we must have

\[
b_{qj} = \sum_{i} \tilde{a}_{qi} c_{ij},
\]

(50)
where the matrix \( C = [c_{ij}] \) is defined via equation (4) for \( N = 2 \). Now we substitute equations (46), (49) and (50) into the expression for the general post-measurement state (equation 48) to obtain the state \( \hat{\Pi}^{(1)}(\rho) \) which easily reduces to

\[
\hat{\Pi}^{(1)}(\rho) = \sum_{ij} (\hat{\Lambda}^{(1)\nu} \hat{\Lambda}^{(1)} C)_{ij} X_{i}^{(1)} \otimes X_{j}^{(2)},
\]

(51)
where \( \hat{\Lambda}^{(1)} \) is the matrix which maximizes \( \text{tr}(A^{(1)} C A^{(1)\nu}) \). Thus, \( \hat{\Pi}^{(1)}(\rho) \) has the form

\[
\hat{\Pi}^{(1)}(\rho) = \sum_{ij} c'_{ij} X_{i}^{(1)} \otimes X_{j}^{(2)}
\]

the same as in equation (4) for \( N = 2 \).

Specializing to two-qubit systems, we have, for \( D_{2}(\hat{\Pi}^{(1)}(\rho)) \), using equation (41),

\[
D_{2}(\hat{\Pi}^{(1)}(\rho)) = \frac{1}{4} (||H||^{2} + ||\hat{\Pi}||^{2} - \zeta_{\text{max}}),
\]

(52)
Clearly, the corresponding post-measurement states are given by discord of these successive measurement states are given by $\rho_{\text{state}} = \text{tr}(I \otimes \sigma_j \tilde{\Pi}^{(1)}(\rho))$, $\tilde{\gamma}_j = \text{tr}(\sigma_i \otimes \sigma_j \tilde{\Pi}^{(1)}(\rho))$, $\tilde{\zeta}_{\text{max}}$ is the largest eigenvalue of the real symmetric matrix $\tilde{\mathcal{G}}^{(2)} = \tilde{\gamma}^{\dagger} + \tilde{\gamma}$ and $\tilde{\Pi}^{(1)}(\rho)$ is given by equation (51). The total quantum correlations in the state $\rho$ are given by

$$Q(\rho) = D_1(\rho) + D_2(\tilde{\Pi}^{(1)}(\rho)))$$

along with equations (40), (52) and (51) (for $\tilde{\Pi}^{(1)}(\rho)$).

6. Total quantum correlations in an $N$-partite state

In this section, we obtain a closed form expression for the total quantum correlations in an $N$-partite quantum state. We use equations (9) and (17).

Consider an $N$-partite state $\rho_{12\cdots N}$ and denote by $\tilde{\Pi}^{(k)}$ the von Neumann measurement minimizing equation (17). It is straightforward to check that the state after the measurement, $\tilde{\Pi}^{(k)}(\rho_{12\cdots N})$, is a zero $k$-discord state, that is, $D_k(\tilde{\Pi}^{(k)}(\rho_{12\cdots N})) = 0$. However, the state $\tilde{\Pi}^{(k)}(\rho_{12\cdots N})$ may have $D_l(\tilde{\Pi}^{(k)}(\rho_{12\cdots N})) \neq 0$, $l \neq k$. Thus, the state $\tilde{\Pi}^{(k)}(\rho_{12\cdots N})$ can have some nonzero quantum correlations. Thus, $D_k(\rho_{12\cdots N})$ cannot give us a measure of the total quantum correlations in the state $\rho_{12\cdots N}$. This analysis suggests a geometric measure of total quantum correlations present in a state $\rho_{12\cdots N}$.

We can now use the above considerations to investigate the total quantum correlations present in a state $\rho_{12\cdots N}$. Let us assume that the non-selective von Neumann projective measurements $\tilde{\Pi}^{(1)}$, $\tilde{\Pi}^{(2)}$, $\ldots$, $\tilde{\Pi}^{(N)}$ are performed successively on $N$ parts $12 \cdots N$, the $k$th successive measurement being performed on the $k$th part, leading to $D_k(\rho_{12\cdots N}) = 0$, where $\rho_{12\cdots N}$ is the state produced after the $(k-1)$th successive measurement, given in equation (54). Clearly, the corresponding post-measurement states are given by

$$\tilde{\Pi}^{(1)}(\rho_{12\cdots N}), \tilde{\Pi}^{(2)}(\rho_{12\cdots N}), \ldots, \tilde{\Pi}^{(N)}(\rho_{12\cdots N}), \ldots.$$ (54)

Here the measurement $\tilde{\Pi}^{(k)}$ minimizes the loss of correlations in the state produced after the first $k-1$ successive measurements on $k-1$ parts. Thus, the geometric measures of quantum discord of these successive measurement states are given by

$$D_1(\rho_{12\cdots N}),$$

$$D_2(\tilde{\Pi}^{(1)}(\rho_{12\cdots N}),$$

$$D_3(\tilde{\Pi}^{(2)}(\rho_{12\cdots N})),$$

$$\vdots$$

$$D_N(\tilde{\Pi}^{(N-1)}(\rho_{12\cdots N})).$$

(58)

Therefore, the geometric measure of total quantum correlations present in an $N$-partite quantum state $\rho_{12\cdots N}$ is given by

$$Q(\rho_{12\cdots N}) = D_1(\rho_{12\cdots N}) + D_2(\tilde{\Pi}^{(1)}(\rho_{12\cdots N})) + D_3(\tilde{\Pi}^{(2)}(\rho_{12\cdots N})) + \cdots + D_N(\tilde{\Pi}^{(N-1)}(\rho_{12\cdots N})).$$

(59)

which is a multipartite generalization of measure (53) introduced in the previous section.

We use equation (9) to write, for the quantum discord $D_k$ corresponding to the $k$th successive measurement on the $k$th part,

$$D_k(\tilde{\Pi}^{(k)}(\rho_{12\cdots N})) = ||\mathcal{C}^{(k)}||^2 - ||\mathcal{C}^{(k)} \times_k \mathcal{A}^{(k)}||^2.$$ (60)
where $A^{(k)}$ gives the maximum value of the second term and the tensor $C^{(k)}$ is defined via equation (4) for the state after the $(k-1)$th measurement. Equation (A.6) in the appendix gives us

$$C^{(k)} = C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})', \quad k = 2, 3, \ldots, N. \quad (61)$$

Therefore, we obtain, for the total quantum correlations $Q(\rho_{12-N})$,

$$Q(\rho_{12-N}) = ||C^{(1)}||^2 - ||C^{(1)} \times_1 \hat{A}^{(1)}||^2 + \sum_{k=2}^{N} ||C^{(k)} \times_{k-1} (\widehat{A}^{(k-1)})'||^2$$

$$-||C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})' \times_k \widehat{A}^{(k-1)}||^2. \quad (62)$$

Written explicitly, the $k$th term in the expression of $Q(\rho_{12-N})$ for $2 \leq k \leq N$ is

$$||C^{(1)} \Pi_{j=2}^{k-1} (\widehat{A}^{(j-1)})' ||^2 - ||C^{(1)} \Pi_{j=2}^{k-1} (\widehat{A}^{(j-1)})' \times_k \widehat{A}^{(k-1)} ||^2,$$

where $C^{(1)} = C$ and $\hat{A}^{(1)}$, maximizing the second term in equation (9), correspond to the starting state $\rho_{12-N}$ via equations (4) and (9).

Next we prove that

$$||C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})'||^2 = ||C^{(k-1)}||^2 - ||C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})'||^2, \quad k = 2, \ldots, N.$$

Using the definition of the norm of a tensor as the inner product of a tensor with itself given in [53], we obtain

$$||C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})'||^2 = \langle C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})', C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})' \rangle.$$

We use propositions 3.11 and 3.4(b) in [53] to obtain

$$\langle C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})', C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})' \rangle = \langle C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})', C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})' \rangle$$

$$= \langle C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})', C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})' \rangle$$

$$= \langle C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})', C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})' \rangle.$$

We know that $\hat{A}^{(k)}(\hat{A}^{(k)})' = I, k = 1, \ldots, N$, so that

$$||C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})'||^2 = ||C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})'||^2 = \langle C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})', C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})' \rangle$$

$$= ||C^{(k-1)} ||^2 - ||C^{(k-1)} \times_{k-1} (\widehat{A}^{(k-1)})'||^2. \quad (63)$$

By using this, all the terms except the first and the last term in equation (62) pairwise cancel. Thus, we finally obtain

$$Q(\rho_{12-N}) = ||C||^2 - ||C \times_1 \hat{A}^{(1)} \times_2 \hat{A}^{(2)} \times_3 \cdots \times_{N-1} \hat{A}^{(N-1)} \times_N \hat{A}^{(N)}||^2. \quad (64)$$

This formula applies to an arbitrary $N$-partite quantum state. However, $Q(\rho_{12-N})$ can be actually computed only for an $N$-qubit state, because the matrices $\hat{A}^{(k)}$ as well as the states $\hat{A}^{(k)}(\rho_{12-N}), k = 1, \ldots, N$, can be explicitly constructed in this case, as shown in section 3 and the appendix (equation (A.4)). Further, for $N$-qubit states, this formula can be experimentally implemented, as all the elements of all the matrices can be determined by measuring Pauli operators on individual qubits, without any a priori knowledge of the $N$-qubit state (see section 7).

From proposition 3.4(a) of [53], namely

$$\mathcal{Y} \times_{m} A \times_{n} B = (\mathcal{Y} \times_{m} A) \times_{n} B = (\mathcal{Y} \times_{n} B) \times_{m} A, \quad m \neq n,$$

where $\mathcal{Y} \in \mathbb{R}^{s_{1} \times \cdots \times s_{L}}$ is an $L$-way tensor and $A \in \mathbb{R}^{s_{m} \times s_{n}}$, $B \in \mathbb{R}^{s_{n} \times s_{m}}$ are matrices, it follows that the total quantum correlation is invariant under arbitrary permutation of factors in equation (64) or is invariant under any permutation of order in which the measurements on individual parts are made.
7. Experimental determination of $D_k$

The quantum discord $D_k$ is a simple function of the elements of the correlation tensors occurring in the Bloch representation of the $N$-qubit state $\rho_{1\cdots N}$ (equations (20) and (23)). Each element of such a tensor is the average value of a tensor product of Pauli operators acting on individual qubits, $\sigma_{\alpha_k}(\alpha_k = 1, 2, 3)$. Each $\sigma_{\alpha_k}$ can be measured on the $k$th qubit and the average over the product of the measured values of an appropriate subset of the $\sigma_{\alpha_k}$, $k = 1, \ldots, N$, experimentally determines the values of the corresponding element of the correlation tensor occurring in equation (23). This involves measuring each Pauli operator over a large ensemble of systems, a feature common to all measurements on quantum systems. Thus, we can experimentally determine the values of all elements of all the correlation tensors in equation (23) and hence the value of $D_k$. Note that a detailed a priori knowledge of the state $\rho_{1\cdots N}$ is not required for the experimental determination of $D_k$. Of course, after all the measurements are made, the resulting collection of the measured values of the Pauli operators $\sigma_{\alpha_k}$, $k = 1, \ldots, N$, is enough to reconstruct $\rho_{1\cdots N}$, using the averages over the products of these values [60]. This argument also shows that the total quantum discord in an $N$-qubit state, being a simple function of $\{D_k\}$, $k = 1, \ldots, N$, of the states produced by successive (optimal) measurements on qubits (see section 6), can also be determined experimentally.

The experimental value of the average obtained via the measurement of the Pauli operators is an estimate of its true value. We can use the central limit theorem to find out how well this estimate behaves for a large number of measurements, say $m$, as it becomes Gaussian with mean equal to the empirical value and the standard deviation proportional to $m^{-1/2}$ [60]. These considerations are common to all measurements on quantum systems. In order to get the measurement and computational complexity of obtaining quantum discord in an $N$-qubit state, we note that, for a general $N$-qubit state, the number of elements in the middle term of equation (23) diverges exponentially as $3 \times 4^{N-1}$. However, these elements are computed using the results of three measurements (of three Pauli operators) on each qubit. Thus, the number of measurements per qubit ($= 3$) is independent of the number of qubits $N$. The measurements on individual qubits are carried out in parallel. The total number of measurements on $N$ qubits is $3N$ which is linear in $N$. Therefore, the exponential complexity of determination of $D_k$ is restricted to its computational part (as the number of tensor elements to be computed increases exponentially with $N$) and does not apply to its measurement part which is linear in $N$. Further, the computation of an individual element of correlation tensors in equation (23) (average over the products of experimental values of Pauli operators) is very simple (linear in $N$). Thus, for a general $N$-qubit state, an experimental estimation of $D_k$ is feasible as long as the number of qubits is not too large. (For a ten-qubit system, about $9 \times 10^5$ elements have to be computed.) In such situations, the possibility of the experimental estimation of quantum discord without any a priori knowledge of the state of the quantum system gives a crucial advantage.

8. Summary and comments

To summarize, we obtain generic forms of quantum discord and total quantum correlations in an $N$-partite state and the corresponding exact formulas in the $N$-qubit case. The formulas for the quantum discord and the total quantum correlations in the $N$-qubit case are not only exactly computable using the $N$-qubit quantum state, but can also be experimentally estimated when the $N$-qubit state is not precisely known. States of quantum systems may not be known at some intermediate stage of quantum information processing and deciphering an unknown quantum state is a formidable task. Hence, it is of great advantage if the crucial resources
such as entanglement or quantum discord can be estimated experimentally, without taking recourse to what the quantum state is. The number of quantities required to be measured goes linearly with the system size \( N \), as only three Pauli operators are to be measured on a qubit. The computational complexity of the discord in an \( N \)-qubit state is dominated by that of the middle term in equation (23) which deals with 3 \( \times \) \( 4^{N-1} \) elements (average values of the tensor products of Pauli operators in the \( N \)-qubit state). Thus, computation increases exponentially with system size. This is not a real restriction when \( N \) is small (\( N = 2, 3, 4 \) qubits). Regarding the operational procedure defining the total quantum correlation in an \( N \)-partite state, we note that it accounts for the total quantum correlations between \( N \) parts as no quantum correlations remain, including all possible cuts. However, if one or more parts contain correlated sub-parts and the optimal measurement is a joint measurement (in an entangled basis) on these sub-parts, then the correlations between these sub-parts remain. These correlations may be eliminated by considering the sub-parts as separate parts of the system. We do not lose any generality in this situation because we are concerned with the quantum correlations between the specified \( N \) parts and our formulas account for these correlations. The actual division of the system into subsystems (parts) is dictated by the correlations required for a particular application. Finally, it will be interesting to seek a generalization of this work to include POVMs.

**Acknowledgments**

This work was supported by the BCUD research grant RG-13. ASMH thanks Pune University for the hospitality during his visit when this work was initiated. PSJ thanks Anil Shaji and Sai Vinjanampathy for a useful discussion. We thank A Osterloh for pointing out [58].

**Appendix. Finding the state \( \widetilde{\Pi}^{(k)}(\rho_{12\ldots N}) \)**

In order to find the optimal von Neumann measurement \( \widetilde{\Pi}^{(k)} \) on \( \rho_{12\ldots N} \) which minimizes \( ||\rho_{12\ldots N} - \Pi^{(k)}(\rho_{12\ldots N})||^2 \), we have to find the corresponding orthonormal basis \( \{|z\rangle\} \) in \( H^k \) such that \( \{|\tilde{z}\rangle\} = \{|z\rangle\} \). The expansion of these 1D projectors \( |\tilde{z}\rangle \) in the basis \( \{X_i^{(k)} \colon i = 1, \ldots, d_k^2 \} \) (generators of \( SU(d_k) \)), that is,

\[
|\tilde{z}\rangle \langle \tilde{z}| = \sum_i \tilde{a}_{iz} X_i^{(k)}, \quad i = 1, \ldots, d_k^2,
\]

(A.1)

with

\[
\tilde{a}_{iz} = \langle \tilde{z}| X_i^{(k)} |\tilde{z}\rangle, \quad z = 1, 2, \ldots, d_k; \quad i = 1, 2, \ldots, d_k^2,
\]

must then give the matrix \( \tilde{A}^{(k)} \) which maximizes \( ||C \times \tilde{A}^{(k)}||^2 \) which in turn gives the \( k \)-discord \( D_k(\rho_{12\ldots N}) \).

To obtain the state \( \widetilde{\Pi}^{(k)}(\rho_{12\ldots N}) \), we proceed as follows. As noticed above, the state \( \tilde{\Pi}^{(k)}(\rho_{12\ldots N}) \) is a zero \( k \)-discord state satisfying \( D_k(\tilde{\Pi}^{(k)}(\rho_{12\ldots N})) = 0 \). Hence, \( \tilde{\Pi}^{(k)}(\rho_{12\ldots N}) \) must have the form of classical quantum state as in equation (6). We expand the state \( \rho_{12\ldots N} \) in equation (6) in terms of the basis \( \{X_j^{(1)} \otimes X_j^{(2)} \otimes \ldots \otimes X_j^{(k-1)} \otimes X_j^{(k+1)} \otimes \ldots \otimes X_j^{(N)} \} \) to obtain

\[
p_{z}|\rho_{12\ldots N}\rangle = \sum_{i_1, i_2, \ldots, i_N} b_{i_1i_2\ldots i_N} X_j^{(1)} \otimes X_j^{(2)} \otimes \ldots \otimes X_j^{(k-1)} \otimes X_j^{(k+1)} \otimes \ldots \otimes X_j^{(N)},
\]

(A.2)

\[z = 1, 2, \ldots, d_k; \quad i_m = 1, \ldots, d_k^2; \quad m = 1, 2, \ldots, N,\]
with \( b_{i_1 \cdots i_k} = \text{tr} \left( \rho_1 \rho_2 \cdots \rho_k \right) X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_k}^{(k)} \). We know from theorem 1 that for equation (9) to hold, we must have

\[
b_{i_1 \cdots i_k} = \sum_{i_k} c_{i_1 \cdots i_k} \alpha_{i_k}. \tag{A.3}
\]

Now, we substitute equations (A.1)–(A.3) into the expression for the general post-measurement state (equation (6)),

\[
\chi_k = \sum_{z=1}^{d_2} p_{z_j} |z_j \rangle \langle z_j | \rho_{i_k} |z_j \rangle
\]

and use the definition of the \( n \)-mode product in equation (7) and proposition 3.4(b) in [53] to obtain the state \( \tilde{\Pi}^{(k)}(\rho_{12\cdots N}) \) which easily reduces to

\[
\tilde{\Pi}^{(k)}(\rho_{12\cdots N}) = \sum_{i_{i_1} \cdots i_{i_k}} [C \times_k \left( (\tilde{A}^{(k)})^\dagger \tilde{A}^{(k)} \right)]_{i_{i_1} \cdots i_{i_k}} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_k}^{(N)}, \tag{A.4}
\]

where \( \tilde{A}^{(k)} \) is the matrix which maximizes \( ||C \times_k A^{(k)}||^2 \). Thus, \( \tilde{\Pi}^{(k)}(\rho_{12\cdots N}) \) has the form

\[
\tilde{\Pi}^{(k)}(\rho_{12\cdots N}) = \sum_{i_{i_1} \cdots i_{i_k}} C'_{i_{i_1} \cdots i_{i_k}} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_k}^{(N)} \tag{A.5}
\]

the same as in equation (4). Finally, we note that the tensor \( C \) occurring in the \( k \)-mode product in equation (A.4) corresponds to the state on which the measurement \( \tilde{\Pi}^{(k)} \) is made, via equation (4) or equation (A.5) applied to such a state. This observation leads to the following result. Applying equation (A.4) to the states on which the \((k-1)\)th and \(k\)th successive measurements are made (on the \((k-1)\)th and \(k\)th parts, respectively), we obtain

\[
\tilde{\Pi}^{(k)}(\tilde{\Pi}^{(k-1)} \rho_{k-2}) = \sum_{i_{i_1} \cdots i_{i_k}} [C^{(k-1)} \times_{k-1} \left( (\tilde{A}^{(k-1)})^\dagger \tilde{A}^{(k-1)} \right)]_{i_{i_1} \cdots i_{i_k}} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_k}^{(N)}
\]

and

\[
\tilde{\Pi}^{(k-1)} \rho_{k-2} = \sum_{i_{i_1} \cdots i_{i_k}} [C^{(k-1)} \times_{k-1} \left( (\tilde{A}^{(k-1)})^\dagger \tilde{A}^{(k-1)} \right)]_{i_{i_1} \cdots i_{i_k}} X_{i_1}^{(1)} \otimes X_{i_2}^{(2)} \otimes \cdots \otimes X_{i_k}^{(N)},
\]

where \( \rho_{k-2} \) is the state on which the \((k-1)\)th measurement is made. The comparison of these two equations in the light of the above observation immediately leads to

\[
C = C^{(k-1)} \times_{k-1} \left( (\tilde{A}^{(k-1)})^\dagger \tilde{A}^{(k-1)} \right). \tag{A.6}
\]

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