Qutrit geometric discord

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Properties of the trace norm geometric discord of the system of two qutrits are studied. The geometric discord of qutrit Bell states, Werner states and bound entangled states is computed.

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I. INTRODUCTION

Quantum correlations in finite-dimensional composite systems have been studied intensively in last decades, originally with focus on the simplest systems i.e. qubit systems. Although one can consider in this respect a generic d-level system, so called qutrit, but progress in studying quantum correlations for qutrits is limited, due to the level of complication. Therefore, three-level systems (qutrits) are intensively studied presently. They are interesting for many reasons. First of all, such systems model realistic three-level atoms in which the interference between different radiative transitions is possible, resulting in new kinds of coherence [1]. Quantum dynamics of collective systems of such atoms significantly differ from a dynamics of two-level atoms (see e.g. [2–4]). On the other hand, the theory of quantum correlations between the pairs of such atoms is much more complex than in the case of qubits. Even description of the set of states of a single qutrit is much more complicated then that for qubit states [5]. Moreover, there is no simple necessary and sufficient condition probing entanglement of qutrits. The Peres-Horodecki separability criterion [6,7] is not sufficient for two qutrit system, it only shows that the states that are not positive after partial transposition (NPPT states) are entangled. It turns out that all entangled states can be divided into two classes: free entangled states that can be distilled using local operations and classical communication (LOCC); bound entangled states for which no LOCC strategy can be used to extract pure state entanglement [5]. Since many effects in quantum information depend on maximally entangled pure states, only distillable states can directly be used for quantum communication.

Recently, more general properties of quantum correlations, which go beyond quantum entanglement, have attracted a lot of interest. They arise from the observation that for pure separable states, there exists von Neumann measurements on a part of composite system that do not disturb the state, whereas nonseparable states are always disturbed by such local measurements. Extension of this feature to the mixed states, gives rise to the notion of quantum discord [9–11]. For pure states notion of quantum discord coincides with entanglement, but in the case of mixed states discord and entanglement differ significantly. For example, almost all quantum states have non-vanishing discord and there exist discordant separable mixed states [12].

To evaluate quantum discord at a given state, one can use its geometric measure instead of the original measure proposed in [9]. Such geometric measure of quantum discord is given by a minimal distance of a given state \( \rho \) from the set of states \( \mathcal{P}_A(\rho) \), obtained after any local measurement \( \mathcal{P}_A \) on a part \( A \). The proper choice of a distance measure is crucial. Presently there are three of them in use. The measure proposed in [13] uses a Hilbert-Schmidt norm to define a distance in the set of states. This choice has a technical advantage: the minimization process can be realized analytically for arbitrary two-qubit states. However this measure has some unwanted properties. The most important problem is that it may increase under local operations performed on the unmeasured system [14–16]. It can be cured by the use of the Schatten 1-norm (trace norm) instead, however such defined measure of quantum discord is more difficult to compute [17]. By now, the explicit formula for it is known only in the case of Bell-diagonal states or two-qubit X-states [17–18]. The third measure used for studying the geometric quantum discord is based on the Bures distance [19]. It has nice property that for pure states it is strictly equal to the geometric measure of entanglement.

In this paper, we extend the analysis of trace norm based geometric discord \( D_1 \) to the system of two qutrits. The results known for the two qutrit system are related to the geometric discord based on the Hilbert-Schmidt norm and give information only about two qutrit Werner states [20] and about upper and lower bounds of such discord in the case of bound entangled states [21]. Firstly we compute the form of \( D_1 \) for special class of states with maximally mixed marginals and diagonal correlation matrix. We find that for pure Bell states and qutrit Werner states, the distance of a state \( \rho \) to states \( \mathcal{P}_A(\rho) \) is constant, and one does not need to minimize over all local measurements to compute quantum discord. The value of this distance for the Bell state we use to normalize \( D_1 \) in such a way that for any state \( \rho \)

\[
0 \leq D_1(\rho) \leq 1
\]

and \( D_1(\rho) = 1 \) for maximally entangled state \( \rho \). Then, the normalized quantum discord is computed for a class of qutrit Werner states \( \rho_W \) and we obtain the result that \( D_1(\rho_W) \) is equal to the mixing parameter \( p \) (Sect. IV.B). For other families of
states with maximally mixed marginals, a minimization over all measurements is necessary. This makes the problem of analytic evaluation of qutrit discord extremely difficult. Fortunately, for examples considered in this work, numerical analysis shows that the minimal distance between $\rho$ and $\mathbb{P}_A(\rho)$ is achieved for projective measurement given by standard orthonormal basis in $\mathbb{C}^3$. In this way we can compute trace norm geometric discord for two-parameter family of mixed entangled states (Sect. V.B). In particular, we obtain first known analytic formula giving trace norm quantum discord of bound entangled states.

**II. QUDIT STATE PARAMETRIZATION**

### A. One - qudit parametrization

Let us start our analysis with the general $d$-level quantum system (qudit). To describe the states of qudit, it is convenient to use as a basis in a set of $d \times d$ matrices the hermitian generators of $\text{su}(d)$ algebra and the identity matrix $\mathbb{I}_d$. Let $\lambda_1, \ldots, \lambda_{d^2-1}$ be the generators of $\text{su}(d)$ algebra. The matrices $\lambda_j$ satisfy

$$\text{tr} \lambda_j = 0, \quad \text{tr} \langle \lambda_j \lambda_k \rangle = 2 \delta_{jk}, \quad j, k = 1, \ldots, d^2 - 1$$

and

$$\lambda_j \lambda_k = \frac{2}{d} \delta_{jk} \mathbb{I}_d + \sum_l (\hat{d}_{jkl} + i \hat{f}_{jkl}) \lambda_l$$  \hspace{1cm} (II.1)

where the structure constants $\hat{d}_{jkl}$ and $\hat{f}_{jkl}$ are given by

$$\hat{d}_{jkl} = \frac{1}{4} \text{tr} (\{\lambda_j, \lambda_k\} \lambda_l)$$  \hspace{1cm} (II.2)

and

$$\hat{f}_{jkl} = \frac{1}{4i} \text{tr} (\{\lambda_j, \lambda_k\} \lambda_l)$$  \hspace{1cm} (II.3)

Using the structure constants (II.2) and (II.3) one can introduce the following "star" and "wedge" products in a real linear space $\mathbb{R}^{d^2-1}$. For $m, n \in \mathbb{R}^{d^2-1}$ we define

$$\langle n \star m \rangle_j = \sqrt{\frac{d(d-1)}{2}} \frac{1}{d-2} \sum_{k,l} \hat{d}_{jkl} n_k m_l$$  \hspace{1cm} (II.4)

and

$$\langle n \wedge m \rangle_j = \sqrt{\frac{d(d-1)}{2}} \frac{1}{d-2} \sum_{k,l} \hat{f}_{jkl} n_k m_l$$  \hspace{1cm} (II.5)

Let $\lambda = (\lambda_1, \ldots, \lambda_{d^2-1})$ and

$$\langle n, \lambda \rangle = \sum_j n_j \lambda_j$$  \hspace{1cm} (II.6)

then taking into account (II.1), we obtain

$$\langle n, \lambda \rangle \langle m, \lambda \rangle = \frac{2}{d} \langle n, m \rangle \mathbb{I}_d + \frac{1}{d} \langle n \star m, \lambda \rangle + \frac{i}{d} \langle n \wedge m, \lambda \rangle,$$  \hspace{1cm} (II.7)

where

$$d' = \sqrt{\frac{d(d-1)}{2}} \frac{1}{d-2}.$$

The set of states of $d$-level system can be parametrized as follows (see e.g. [22])

$$\rho = \frac{1}{d} \left( \mathbb{I}_d + d'' \langle n, \lambda \rangle \right), \quad n \in \mathbb{R}^{d^2-1},$$  \hspace{1cm} (II.8)

where

$$d'' = \sqrt{\frac{d(d-1)}{2}}$$

and the components of the vector $n$ are

$$n_j = \frac{d}{\sqrt{2d(d-1)}} \text{tr} (\rho \lambda_j), \quad j = 1, \ldots, d^2 - 1.$$

The matrix (II.8) is hermitian and has a unit trace. To describe a quantum state, the matrix $\rho$ have to be positive-definite and this condition is not easy to characterize in terms of the vector $n$. However the pure states given by one-dimensional projectors can be fully described. Using (II.7), one can check that $\rho$ given by (II.8) satisfies $\rho^2 = \rho$ if and only if

$$\langle n, n \rangle = 1 \quad \text{and} \quad n \star n = n.$$

### B. Two - qudit parametrization

Consider now two qudits $A$ and $B$. The state of a compound system can be parametrized as follows

$$\rho = \frac{1}{d^2} \left( \mathbb{I}_d \otimes \mathbb{I}_d + d'' \langle x, \lambda \rangle \otimes \mathbb{I}_d + \mathbb{I}_d \otimes d'' \langle y, \lambda \rangle ight) + \sum_{j,k=1}^{d^2-1} T_{jk} \lambda_j \otimes \lambda_k$$  \hspace{1cm} (II.9)

with $x, y \in \mathbb{R}^{d^2-1}$. Notice that

$$x_j = \frac{d}{\sqrt{2d(d-1)}} \text{tr} (\rho \lambda_j \otimes \mathbb{I}_d), \quad y_j = \frac{d}{\sqrt{2d(d-1)}} \text{tr} (\rho \mathbb{I}_d \otimes \lambda_j)$$

and

$$T_{jk} = \frac{d^2}{4} \text{tr} (\rho \lambda_j \otimes \lambda_k).$$

The parametrization (II.9) is chosen is such a way, that the marginals $\text{tr}_B \rho$ and $\text{tr}_A \rho$ are given by the vectors $x$ and $y$ as in (II.8).
III. TRACE-NORM GEOMETRIC QUDIT DISCORD

When a bipartite system $\mathcal{AB}$ is prepared in a state $\rho$ and we perform local measurement on the subsystem $\mathcal{A}$, almost all states $\rho$ will be disturbed due to such measurement. The one-sided geometric discord is defined as the minimal disturbance induced by any projective measurement $\mathbb{P}_A$ on subsystem $\mathcal{A}$ [13]. Here we choose a distance in the set of states given by the trace norm, instead of Hilbert-Schmidt norm used in the standard approach, and define (not normalized) measure of quantum discord as [12]

$$\bar{D}_1(\rho) = \min_{\mathbb{P}_A} ||\rho - \mathbb{P}_A(\rho)||_1,$$  \hspace{1cm} (III.1)

where

$$||\sigma||_1 = \text{tr} |\sigma|.$$

In the case of qubits, local projective measurement $\mathbb{P}_A$ is given by the one-dimensional projectors $P_1, P_2, \ldots, P_d$ on $\mathbb{C}^d$, such that

$$P_1 + P_2 + \cdots + P_d = \mathbb{I}_d, \quad P_i P_k = \delta_{jk} P_k$$

and $\mathbb{P}_A = \mathbb{P} \otimes \text{id}$, where

$$\mathbb{P}(\sigma) = P_1 \sigma P_1 + P_2 \sigma P_2 + \cdots + P_d \sigma P_d.$$

It is worth to stress that definition (III.1) is equivalent to the more common one, which is given by the minimal distance of a given state to the set $\Omega_0$ of all states with zero discord. In the case of one-sided quantum discord studied in this paper, the set $\Omega_0$ contains all “classical-quantum” states

$$\rho_{cq} = \sum_{k=1}^d p_k |\psi_k\rangle \langle \psi_k| \otimes \rho^{B}_k,$$

where $\{\psi_k\}$ is any single-qutrit orthonormal basis, $\{\rho^{B}_k\}$ are any states of the subsystem $B$ and $p_k \geq 0$, $\sum_{k=1}^d p_k = 1$.

For the state (II.9) we have

$$\rho - \mathbb{P}_A(\rho) = \frac{1}{d^2} \left[ d'^2 \langle x, \lambda \rangle - \mathbb{P}(d'^2 \langle x, \lambda \rangle) \otimes \mathbb{I}_d + \sum_{j,k=1}^{d^2-1} T_{jk} (\lambda_j - \mathbb{P}(\lambda_j)) \otimes \lambda_k \right].$$

Since

$$\mathbb{P}(\lambda_j) = \sum_{k=1}^{d^2-1} a_{jk} \lambda_k, \quad a_{jk} = \frac{1}{2} \text{tr} \left( \mathbb{P}(\lambda_j) \lambda_k \right)$$

and the matrix $A = (a_{jk})$ is real and symmetric (in fact it is a projector operator [23]),

$$\mathbb{P}(\langle m, \lambda \rangle) = \langle m, A \lambda \rangle = \langle Am, \lambda \rangle, \quad m \in \mathbb{R}^{d^2-1}.$$  

So

$$\rho - \mathbb{P}_A(\rho) = \frac{1}{d^2} \left[ d'^2 \langle M_x, \lambda \rangle \otimes \mathbb{I}_d + \sum_{j,k} T_{jk} \langle Me_j, \lambda \rangle \otimes \langle e_k, \lambda \rangle \right]$$

where $M = \mathbb{I}_d - A$ and $\{e_j\}_{j=1}^{d^2-1}$ is the canonical basis in $\mathbb{R}^{d^2-1}$. Let $R(M)$ denotes the right side of equation (III.2). Then not normalized geometric quantum discord of the state (II.9) equals

$$\bar{D}_1(\rho) = \min_M ||R(M)||_1 = \min_M \text{tr} \sqrt{Q(M)}$$  \hspace{1cm} (III.3)

where $Q(M) = R(M) R(M)^*$ and the minimum is taken over all matrices $M$ corresponding to a measurements on subsystem $\mathcal{A}$.

To simplify further computations, we consider first the states with maximally mixed marginals i.e. such states $\rho$ that

$$\text{tr}_B \rho = \frac{\mathbb{I}_d}{d}, \quad \text{tr}_A \rho = \frac{\mathbb{I}_d}{d}.$$  \hspace{1cm} (III.4)

In the parametrization (II.9) this property corresponds to $x = y = 0$. We also choose such states for which the correlation matrix $T = (T_{jk})$ is diagonal. (Notice that contrary to the case of qubits $d = 2$, the general state of two qudits $d > 2$ satisfying (III.4) is not locally equivalent to the state with diagonal $T$ and such defined class is only a subclass of all states with maximally mixed marginals.) Let

$$T = \text{diag}(t_1, \ldots, t_{d^2-1}),$$

then

$$R(M) = \frac{1}{d^2} \sum_{j=1}^{d^2-1} t_j \langle Me_j, \lambda \rangle \otimes \langle e_j, \lambda \rangle,$$  \hspace{1cm} (III.5)

and using (II.7), we obtain

$$Q(M) = \frac{1}{d^2} \left[ 4 \sum_j t_j^2 \langle Me_j, Me_j \rangle \mathbb{I}_d \mathbb{I}_d + \frac{2}{d^2} \sum_j t_j \langle Me_j, Me_j \rangle \mathbb{I}_d \otimes \langle e_j, e_k \rangle + \frac{1}{d^2} \sum_{j,k} t_{jk} \langle Me_j, Me_k \rangle \mathbb{I}_d \otimes \langle e_j, e_k \rangle \right].$$

IV. THE CASE OF QUTRITS

Now we consider in more details the case of two qudits i.e. when $d = 3$. In this case $d' = d'' = \sqrt{3}$ and the set of projectors corresponding to local projective measurement forms the four
parameter family. In the explicit parametrization we have (see e.g. [24])

\[
P_1 = \begin{pmatrix}
\cos^2 \theta \sin^2 \varphi & e^{-i(\psi - \chi)} a(\theta, \varphi) e^{i \frac{\theta}{2} b(\theta, \varphi)} \\
e^{-i(\psi - \chi)} a(\theta, \varphi) & \sin^2 \theta \sin^2 \varphi & e^{i \gamma} c(\theta, \varphi) \\
e^{-i \gamma} b(\theta, \varphi) & -e^{-i \gamma} c(\theta, \varphi) & \cos^2 \varphi
\end{pmatrix},
\]

\[
P_2 = \begin{pmatrix}
\cos^2 \theta \cos^2 \varphi & e^{-i(\psi - \chi)} d(\theta, \varphi) - e^{i \psi} b(\theta, \varphi) \\
e^{i(\psi - \chi)} d(\theta, \varphi) & \sin^2 \theta \cos^2 \varphi & -e^{i \gamma} c(\theta, \varphi) \\
e^{i \gamma} b(\theta, \varphi) & -e^{-i \gamma} c(\theta, \varphi) & \sin^2 \varphi
\end{pmatrix},
\]

\[
P_3 = \begin{pmatrix}
\sin^2 \theta & -\frac{1}{2} e^{-i(\psi - \chi)} \sin 2 \theta & 0 \\
0 & \cos^2 \theta & 0
\end{pmatrix},
\]

where

\[
a(\theta, \varphi) = \frac{1}{2} \sin 2 \theta \sin^2 \varphi,
\]

\[
b(\theta, \varphi) = \frac{1}{2} \cos \theta \sin 2 \varphi,
\]

\[
c(\theta, \varphi) = \frac{1}{2} \sin \theta \sin 2 \varphi,
\]

\[
d(\theta, \varphi) = \frac{1}{2} \sin 2 \varphi \cos^2 \theta.
\]

and \( \theta, \varphi, \chi \in [-\pi, \pi], \psi \in [-\pi/2, \pi/2]. \)

Our first attempt is to compute quantum discord for states with diagonal correlation matrix \( T \) and matrix elements

\[
t_j = t \varepsilon_j, \quad j = 1, \ldots, 8,
\]

where

\[
\varepsilon_j = \begin{cases}
+1, & j = 1, 3, 4, 6, 8 \\
-1, & j = 2, 5, 7
\end{cases}.
\]

This kind of correlation matrix corresponds for example to qutrit Bell states and Werner states. Notice that in this case

\[
\sum_{j,k} t_j t_k \langle \varepsilon_j, \varepsilon_k \rangle \|3 \otimes \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle
\]

\[
= t^2 \sum_{j,k} \varepsilon_j \varepsilon_k \langle \varepsilon_j, \varepsilon_k \rangle \|3 \otimes \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle
\]

\[
= t^2 \sum_{j,k} \langle \varepsilon_j, IMI e_k \rangle \|3 \otimes \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle,
\]

where

\[
I = \text{diag} (\varepsilon_1, \ldots, \varepsilon_8).
\]

Since

\[
\sum_j \langle \varepsilon_j, IMI e_k \rangle \|3 \otimes \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle
\]

\[
= \|3 \otimes (\sum_j \langle \varepsilon_j, IMI e_k \rangle e_j \ast e_k, \lambda)
\]

\[
= \|3 \otimes (IMI e_k \ast e_k, \lambda),
\]

the sum (IV.2) is equal to

\[
t^2 \|3 \otimes \sum_k \langle IMI e_k \ast e_k, \lambda \rangle.
\]

By a direct computation one can check that

\[
\sum_k IMI e_k \ast e_k = 0,
\]

so also the sum (IV.2) is equal to zero. Moreover, since

\[
\sum_j IMI e_j \ast IMI e_j = 0,
\]

we have

\[
\sum_{j,k} t^2 \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle \|3 = 0.
\]

Notice that

\[
\sum_{j=1}^8 \langle \varepsilon_j, \varepsilon_j \rangle = \sum_{j=1}^8 \langle \varepsilon_j, \varepsilon_j \rangle = \text{tr} M,
\]

so

\[
Q(M) = \frac{1}{8} \left[ \frac{4t^2}{9} \text{tr} M \|3 \otimes \|3 + \frac{1}{3} \sum_{j,k=1}^8 t_j t_k \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle \otimes \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle - \frac{1}{3} \sum_{j,k=1}^8 t_j t_k \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle \otimes \langle \varepsilon_j \ast \varepsilon_k, \lambda \rangle \right]
\]

and

\[
\text{tr} Q(M) = \frac{4t^2}{9} \text{tr} M \cdot \text{tr} \|3 \cdot \text{tr} \|3 = \frac{4t^2}{81} \text{tr} M.
\]

Since \( M = \|8 - A \) projects on six-dimensional subspace of \( \mathbb{R}^8 \), \( M = 6 \) and

\[
\text{tr} Q(M) = \left( \frac{2}{3} \right)^3 t^2.
\]

By the similar, but more involved computations, one can check that

\[
\text{tr} Q(M)^k = q_k t^{2k}, \quad k = 2, \ldots, 9,
\]

where \( q_k \) are constants. In particular

\[
\text{tr} Q(M)^k = \text{tr} Q(M^0)^k, \quad k = 1, \ldots, 9,
\]

where \( M_0 \) denotes the matrix \( M \) with all parameters equal to zero. From that, it follows that the eigenvalues of \( Q(M) \) and \( Q(M_0) \) are the same [25] and the distance between \( \rho \) and \( \mathbb{P}_d (\rho) \) is constant. Thus for such class of states to compute quantum discord we need not to minimize over all matrices \( M \) and it is enough to find the trace norm of \( \sqrt{Q(M_0)} \). Next we consider two examples of states with the correlation matrix satisfying (IV.1).
A. Qutrit Bell state

We start with the Bell state of two qutrits i.e the maximally entangled pure state given by the vector

\[ \Psi_0 = \frac{1}{\sqrt{3}} \sum_{k=1}^{3} \varphi_k \otimes \varphi_k, \]

where \( \{ \varphi_k \} \) is the standard orthonormal basis in \( \mathbb{C}^3 \). The correlation matrix corresponding to this state is given by

\[ T = \text{diag} \left( \frac{3}{2}, -\frac{3}{2}, 0, 0, 0, 0, 0, 0, 0, 0 \right). \]

One can check that in this case

\[ Q(M_0) = \frac{1}{9} \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \]

and

\[ \text{sp} Q(M_0) = \left\{ \frac{4}{9}, \frac{1}{9}, \frac{1}{9}, 0, 0, 0, 0, 0, 0, 0 \right\}, \]

so

\[ \tilde{D}_1(\Psi_0) = \text{tr} \sqrt{Q(M_0)} = \frac{4}{3}. \]

It is natural to demand that the quantum discord of any maximally entangled state be equal to 1, so we introduce normalized geometric measure of qutrit discord \( D_1(p) \), defined as

\[ D_1(p) = \frac{3}{4} \tilde{D}_1(p). \]

Obviously \( D_1(\Psi_0) = 1 \).

B. Qutrit Werner states

As a second example we shall consider the family of qutrit Werner states

\[ \rho_W = (1 - p) \frac{1}{9} + p |\Psi_0\rangle \langle \Psi_0|, \quad p \in [0, 1]. \]  

(IV.4)

The states (IV.4) have interesting properties. For \( p \leq 1/4 \), \( \rho_W \) are PPT states, whereas for \( p > 1/4 \) they are NPPT. In fact such Werner states are distillable, since they violate reduction criterion of separability [26].

One can check that in this case

\[ T = \text{diag} \left( \frac{3}{2}p, -\frac{3}{2}p, \frac{3}{2}p, \frac{3}{2}p, -\frac{3}{2}p, -\frac{3}{2}p, -\frac{3}{2}p, -\frac{3}{2}p, \frac{3}{2}p, \frac{3}{2}p \right) \]

so the corresponding matrix \( Q(M_0) \) is just the matrix (IV.3) multiplied by the factor \( p \) and

\[ D_1(\rho_W) = p. \]

It is instructive to compare just obtained measure of quantum discord with other measures of quantum correlations. First consider Hilbert -Schmidt norm geometric discord \( D_2(p) \), which in the case of two qutrits is defined as (see e.g [27])

\[ D_2(p) = \min_{p, \sigma} \frac{3}{2} ||p - \mathbb{P}_2(p)||^2_2, \]

where

\[ ||\sigma||_2^2 = \text{tr}(\sigma \sigma^*). \]

For the states considered in this subsection

\[ D_2(\rho_W) = \frac{3}{2} \text{tr} Q(M) = \frac{4}{9} r^2. \]

In particular, for the Werner state

\[ D_2(\rho_W) = p^2, \]  

(IV.5)

and

\[ D_1(\rho_W) = \sqrt{D_2(\rho_W)}. \]

The result (IV.5) was previously obtained in [20], where the authors used minimization over all local measurements, which as we have shown, is not needed.

Now we discuss the relation between \( D_1 \) and the measure of entanglement given by negativity, which in the case of two-qutrits is defined as [28]

\[ N(p) = \frac{1}{2} (||p^{PT}||_1 - 1), \]

where \( p^{PT} \) denotes partial transposition of the state \( p \). If \( N(p) > 0 \) then the state \( p \) is non separable, but negativity cannot detect bound entangled states. For the Werner state we have

\[ N(\rho_W) = \begin{cases} 0, & p \leq \frac{1}{4} \\ \frac{1}{2}(4p - 1), & p > \frac{1}{4} \end{cases}. \]

Obviously

\[ D_1(\rho_W) \geq N(\rho_W) \]

which is in accordance with the general result proved in [29].
V. OTHER EXAMPLES

A. Some states with diagonal correlation matrix

Now we consider the family of states with more general diagonal matrix \( T \), not satisfying the condition (V.1). Let

\[
\rho = \begin{pmatrix}
\frac{1}{2} & 0 & 0 & 0 & \alpha & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
an & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & c \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & c & 0 & 0 & 0 & \frac{1}{2}
\end{pmatrix},
\]

where \( a \geq 0, c \geq 0 \). The matrix (V.1) is positive-definite if and only if \( a^2 + c^2 \leq 1/9 \), so in polar coordinates we have

\[
a = r \cos \theta, \quad c = r \sin \theta, \quad r \in [0, 1/3], \quad \theta \in [0, \pi/2].
\]

The corresponding correlation matrix is given by

\[
T = \text{diag} \left( \frac{9}{2} a, -\frac{9}{2} a, \frac{3}{2}, 0, \frac{9}{2} c, -\frac{9}{2} c, \frac{3}{2} \right).
\]

In this case the distance between \( \rho \) and \( \mathcal{P}_M(\rho) \) is not constant and to compute \( D_1(\rho) \) we must minimize \( \text{tr} \sqrt{Q(M)} \) over all projectors \( M \). However numerical computations show that the minimum is achieved for \( M = M_0 \). Since

\[
Q(M_0) = \begin{pmatrix}
\alpha^2 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha c \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a^2 + c^2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\alpha c & 0 & 0 & 0 & 0 & 0 & 0 & c^2
\end{pmatrix},
\]

and

\[
\text{sp} \ Q(M_0) = \{ \alpha^2 + c^2, a^2 + c^2, 0, 0, 0, 0, 0, 0 \},
\]

we have

\[
D_1(\rho) = \frac{3}{2} \sqrt{a^2 + c^2} = \frac{3}{2} r.
\]

On the other hand

\[
N(\rho) = a + c = r (\cos \theta + \sin \theta)
\]

and obviously

\[
D_1(\rho) > N(\rho).
\]

B. States with non-diagonal correlation matrix: bound entangled states

Let us finally consider the following family of states [30]

\[
\rho_\alpha = \frac{2}{7} |\Psi_0\rangle \langle \Psi_0| + \frac{\alpha}{7} \rho_+ + \frac{5 - \alpha}{7} \rho_-,
\]

where

\[
\rho_+ = \frac{1}{3} \left[ P_{\Psi_1 \otimes \Psi_2} + P_{\Psi_2 \otimes \Psi_3} + P_{\Psi_3 \otimes \Psi_1} \right]
\]

\[
\rho_- = \frac{1}{3} \left[ P_{\Psi_2 \otimes \Psi_1} + P_{\Psi_3 \otimes \Psi_2} + P_{\Psi_1 \otimes \Psi_3} \right]
\]

and \( 0 \leq \alpha \leq 5 \). It is known that the states (V.2) are separable for \( 2 \leq \alpha \leq 3 \), bound entangled for \( 3 < \lambda \leq 4 \) and free entangled for \( 4 < \lambda \leq 5 \). One can check that the marginals of \( \rho_\alpha \) are maximally mixed, but the correlation matrix \( T \) is not diagonal. In fact \( T \) equals to

\[
\begin{bmatrix}
3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -\frac{4}{3} & 0 & 0 & 0 & \frac{3\sqrt{3}}{4}(2\alpha - 5) \\
1 & 7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & -3 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3}{4}
\end{bmatrix}
\]

In this case we have to use directly the formula (H.12). As in the previous example, numerical computations show that it is enough to consider \( Q(M_0) \), which is equal to

\[
Q(M_0) = \frac{4}{441} \begin{pmatrix}
2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 2 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 2
\end{pmatrix},
\]

So we have

\[
D_1(\rho_\alpha) = \frac{3}{4} \text{tr} \sqrt{Q(M_0)} = \frac{2}{7}
\]

and we see that quantum discord does not discriminate between separable, bound entangled and free entangled states. On the other hand \( D_1(\rho_\alpha) > N(\rho_\alpha) \), where

\[
N(\rho_\alpha) = \begin{cases}
\frac{1}{2} \left( G(\alpha) - 5 \right), & \alpha \in [0, 1] \cup [4, 5] \\
0, & \alpha \in (1, 4)
\end{cases}
\]

with

\[
G(\alpha) = \sqrt{41 - 20\alpha + 4\alpha^2}.
\]
We can also simply compute Hilbert-Schmidt quantum discord. It is equal to

$$D_2(\rho_\alpha) = \frac{3}{2} \text{tr} Q(M_0) = \frac{4}{49},$$

so

$$D_1(\rho_\alpha) = \sqrt{D_2(\rho_\alpha)}.$$

To the authors best knowledge, the above results are the first exact results giving quantum discord of bound entangled states. The earlier known result concerns Hilbert-Schmidt quantum discord and provides only the lower and upper bounds for $D_2(\rho_\alpha)$ [21]. In particular it was shown that

$$D_2(\rho_\alpha) \geq \begin{cases} \frac{4}{49}, & \alpha \in [0, \alpha_-] \cup [\alpha_+, 5] \\ \frac{4}{49} (9 - 5\alpha + \alpha^2), & \alpha \in (\alpha_-, \alpha_+) \end{cases} \quad (V.5)$$

and the bound (V.5) is consistent with the obtained value of $D_1(\rho_\alpha)$.

The family of states (V.2) is interesting also for another reason. When we have non-diagonal correlation matrix $T$, we can always apply to it singular value decomposition

$$T = V_T W,$$

where $V, W$ are orthogonal matrices and

$$T_0 = \text{diag}(s_1, s_2, \ldots, s_{d^2-1}),$$

with matrix elements $s_k$ given by singular values of $T$. In the case of qubits ($d = 2$), this procedure always leads to locally equivalent states, so we can restrict the analysis to the case of diagonal correlation matrix. For qubits it is generally not true and the states (V.2) are the explicit counterexamples. To show this, we notice that the singular values of the correlation matrix of the states (V.2) are given by

$$s_1 = \cdots = s_6 = \frac{3}{7}, s_7 = s_8 = \frac{3}{28} \sqrt{1 + 3(2\alpha - 5)^2}.$$ (V.6)

Then we take $T_0$ defined by the sequence (V.6) and try to construct a state using the formula (II.9), but we end with the matrix which not positive-definite. Thus there is no equivalent description of the family (V.2) by the states with diagonal correlation matrices.

VI. CONCLUSIONS

We have studied behaviour of the geometric discord based on the trace norm in the system of two qutrits. Analysis of such a system is the first non-trivial step in extending the two-qubit theory of quantum correlations to the general case of $d$-level systems. We have computed geometric discord for some interesting families of two-qutrit states, such as maximally entangled Bell states, Werner states and bound entangled states. Our analysis of qutrit systems in which entanglement can be bound or free, show, even more clearly then in the qubit case, that discord and entanglement describe different aspects of quantum correlations in composed systems.

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