On correlations and mutual entropy
in quantum composite systems

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Abstract
We study the correlations of classical and quantum systems from the information theoretical points of view. We analyze a simple measure of correlations based on entropy (such measure was already investigated as the degree of entanglement by Belavkin, Matsuoka and Ohya). Contrary to naive expectation, it is shown that separable state might possess stronger correlation than an entangled state.

1 Introduction
Correlations play a key role both in classical and quantum physics. In particular the study of correlations is crucial in many-body physics and classical and quantum statistical physics. Recently, it turned out that correlations play prominent role in quantum information theory and many modern applications of quantum technologies and there are dozens of papers dealing with this problem (for the recent review see e.g. [27]).

The aim of this paper is to analyze classical and quantum correlations encoded in the bi-partite quantum states. Beside quantum entanglement we analyze a new measure – so called $D$-correlations – and the quantum discord. We propose to compare correlations of different bi-partite states with the same reduces states, i.e. locally they contain the same information. It is shown that surprisingly a separable state may be more correlated that an entangled one. Analyzing simple examples of Bell diagonal states we illustrate the behavior of various measures of correlations. We also provide an introduction to bi-partite states and entanglement mappings introduced by Belavkin and Ohya and recall basic notions from classical and quantum information theory. An entanglement mapping encodes the entire information about a bi-partite quantum state and hence it provides an interesting way to deal with entanglement theory. Interestingly, it may be applied in infinite-dimensional case and in the abstract $C^*$-algebraic settings. Therefore, in a sense, it provides a universal tool in entanglement theory.

The paper is organized as follows: in the next section we recall basic facts from the theory of composite quantum systems and introduce the notion of entanglement mappings. Moreover, we recall an interesting construction of quantum conditional probability operators. Section 3 recalls classical and quantum entropic quantities and collects basic facts from classical and quantum information theory. In particular it contains the new measure of correlation called $D$-correlation. Section 4 recalls the notion of quantum discord which was intensively analyzed recently in the literature. In section 5 we recall the notion of a circulant state and provide several examples of states for which one is able to compute various measures of correlations. Final conclusions are collected in the last section.

Throughout the paper, we use standard notation: $H$, $K$ for complex separable Hilbert spaces and denote the set of the bounded operators and the set of all states on $H$ by $B(H)$ and $S(H)$, respectively. In the
$d$-dimensional Hilbert space, the standard basis is denoted by $\{e_0, e_1, \cdots, e_{d-1}\}$ and the inner product is denoted by $\langle \cdot, \cdot \rangle$. We write $e_j$ for $|e_j \rangle \langle e_j |$. Given any state $\theta$ on the tensor product Hilbert space $\mathcal{H} \otimes \mathcal{K}$, we denote by $\text{Tr}_K \theta$ the partial trace of $\theta$ with respect to $\mathcal{K}$.

2 Quantum states and entanglement maps

Consider a quantum system living in the Hilbert space $\mathcal{H}$. In this paper we consider only finite dimensional case. However, as we shall see several results may be nicely generalized to the infinite-dimensional setting. Denote by $\mathcal{T} (\mathcal{H})$ a set of trace class operators in $\mathcal{H}$, meaning that $\rho \in \mathcal{T} (\mathcal{H})$ if $\rho \geq 0$ and $\text{Tr} \rho < \infty$, which is always true in finite-dimensional case. Finally, let

$$\mathcal{S}(\mathcal{H}) = \{\rho \in \mathcal{T}(\mathcal{H}) \mid \text{Tr} \rho = 1\},$$

Consider now a composite system living in $\mathcal{H} \otimes \mathcal{K}$ and denote by $\mathcal{S}_{\text{SEP}} \subset \mathcal{S}(\mathcal{H} \otimes \mathcal{K})$ a convex subset of separable states in $\mathcal{H} \otimes \mathcal{K}$. Recall that $\rho \in \mathcal{S}(\mathcal{H} \otimes \mathcal{K})$ is separable if $\rho = \sum_{\alpha} p_{\alpha} \eta_{\alpha} \otimes \sigma_{\alpha}$, where $\eta_{\alpha} \in \mathcal{S}(\mathcal{H})$ and $\sigma_{\alpha} \in \mathcal{S}(\mathcal{K})$, and $p_{\alpha}$ denotes probability distribution: $p_{\alpha} \geq 0 \text{ and } \sum_{\alpha} p_{\alpha} = 1$. A state $\rho \in \mathcal{S}(\mathcal{H} \otimes \mathcal{K})$ is called positive partial transpose (PPT) if its partial transpose satisfies $(\text{id}_{\mathcal{H}} \otimes \tau) \rho \geq 0$, where $\text{id}_{\mathcal{H}}$ denotes an identity map in $\mathcal{B}(\mathcal{H})$. It means that $\rho$ is PPT if $(\text{id}_{\mathcal{H}} \otimes \tau) \rho \in \mathcal{S}(\mathcal{H} \otimes \mathcal{K})$. Denote by $\mathcal{S}_{\text{PPT}}$ a convex subset of PPT states. It is well known [41] that $\mathcal{S}(\mathcal{H} \otimes \mathcal{K}) \supset \mathcal{S}_{\text{PPT}} \supset \mathcal{S}_{\text{SEP}}$. In general, the PPT condition is not sufficient for separability.

Interestingly, due to the well known duality between states living in $\mathcal{H} \otimes \mathcal{K}$ and linear maps $\mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$, one may translate the above setting in terms of linear maps. Let us recall basic facts concerning completely positive maps [40]. A linear map $\chi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ is said to be completely positive (CP) if, for any $n \in \mathbb{N}$, the map

$$\chi_n : M_n(\mathbb{C}) \otimes \mathcal{B}(\mathcal{K}) \longrightarrow M_n(\mathbb{C}) \otimes \mathcal{B}(\mathcal{H}), \quad (a_{i,j})_{i,j} \longrightarrow \left( \chi(a_{i,j}) \right)_{i,j}$$

(2.1)

is positive, where $\mathcal{B}(\mathcal{H})$ denotes bounded operators in $\mathcal{H}$ and $M_n(\mathbb{C})$ stands for $n \times n$ matrices with entries in $\mathbb{C}$. A linear map $\chi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ is said to be completely copositive (CCP) if composed with transposition $\tau$, i.e. $\tau \circ \chi$, is CP.

Consider now a state $\theta \in \mathcal{S}(\mathcal{H} \otimes \mathcal{K})$ and let $\phi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ be a linear map defined by

$$\phi(b) := \text{Tr}_K \left[ (1_{\mathcal{H}} \otimes b) \theta \right],$$

for any $b \in \mathcal{B}(\mathcal{K})$. The dual map $\phi^*$ reads

$$\phi^*(a) = \text{Tr}_H \left[ (a \otimes 1_{\mathcal{K}}) \theta \right],$$

for any $b \in \mathcal{B}(\mathcal{H})$. It should be stressed that the above construction is perfectly well defined also in the infinite-dimensional case if we assume that $\theta$ is a normal state, that is, it is represented by the density operator. Note, that a state $\theta$ and the linear map $\phi$ give rise a linear functional $\omega : \mathcal{B}(\mathcal{H} \otimes \mathcal{K}) \to \mathbb{C}$

$$\omega(a \otimes b) := \text{Tr}(a \otimes b) \theta,$$

(2.2)

for any $a \in \mathcal{B}(\mathcal{H})$, $b \in \mathcal{B}(\mathcal{K})$. This formula may be equivalently rewritten as follows

$$\omega(a \otimes b) = \text{Tr}_H a \phi(b) = \text{Tr}_K \phi^*(a) b.$$  

(2.3)

It is clear that the marginal states read

$$\text{Tr}_K \theta = \phi(1_{\mathcal{K}}) \in \mathcal{B}(\mathcal{H}), \quad \text{Tr}_H \theta = \phi^*(1_{\mathcal{H}}) \in \mathcal{B}(\mathcal{K}).$$

(2.4)

Belavkin and Ohya observed [11][12] that if $\theta \in \mathcal{S}(\mathcal{H} \otimes \mathcal{K})$, then both $\phi$ and its dual $\phi^*$ are CCP. We denote by $\mathcal{B}(\mathcal{H})$ the dual space to the algebra $\mathcal{B}(\mathcal{H})$.

**Definition 2.1** A CCP map $\phi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H})$ normalized as $\text{Tr}_H \phi(1_{\mathcal{K}}) = 1$ is called the entanglement map from $\rho := \phi^*(1_{\mathcal{H}}) \in \mathcal{B}(\mathcal{K})$ to $\sigma := \phi(1_{\mathcal{K}}) \in \mathcal{B}(\mathcal{H})$.

A density operator $\theta_\phi$ corresponding to the entanglement map $\phi$ with its marginals $\phi^*(1_{\mathcal{H}})$ and $\phi(1_{\mathcal{K}})$ can be represented as follows: let $\psi^*_\phi$ denotes a maximally entangled state in $\mathcal{K} \otimes \mathcal{K}$. Then

$$\theta_\phi := (\phi \otimes \tau) P^+_{\phi},$$

(2.5)
with \( P^+_K = d_K |\varphi^+_K\rangle \langle \varphi^+_K| \), where \( d_K = \dim K \). If \( \{e_k\} \) stands for an orthonormal basis in \( K \), then
\[
P^+_K = \sum_{i,j=1}^{d_K} e_{ij} \otimes e_{ij}, \tag{2.6}
\]
with \( e_{ij} := |e_i\rangle \langle e_j| \), and hence
\[
\theta_\phi = \sum_{i,j=1}^{d_K} \phi(e_{ij}) \otimes e_{ij}. \tag{2.7}
\]
The map assigning \( \theta_\phi \) to \( \phi \) is usually called a Choi-Jamiołkowski isomorphism. It should be stressed that \( \theta_\phi \) does not depend upon the choice of \( \{e_k\} \).

**Lemma 2.2** A linear map \( \phi : \mathcal{B}(K) \rightarrow \mathcal{B}(H) \) is CCP if and only if \( \theta_\phi \geq 0 \). Clearly, \( \phi \) is CP if and only if \( \phi \circ \tau \) is CCP.

Due to Lemma 2.2 we have the following criterion.

**Theorem 2.3** \([29, 32]\) A state \( \theta_\phi \) is a PPT state if and only if its entanglement map \( \phi \) is CP.

Recently, Kossakowski et al.\([5]\) proposed the following construction: for \( \theta \in \mathcal{S}(H \otimes K) \) one defines the bounded operator
\[
\pi_\theta := (\rho^{-\frac{i}{2}} \otimes 1_K) \theta (\rho^{-\frac{i}{2}} \otimes 1_K), \tag{2.8}
\]
where \( \rho := \text{Tr}_K \theta \). It is verified that \( \pi_\theta \) satisfies
\[
\pi_\theta \geq 0, \tag{2.9}
\]
\[
\text{Tr}_K \pi_\theta = 1_H \in \mathcal{B}(H). \tag{2.10}
\]
In what follows we assume that \( \rho \) is a faithful state, i.e. \( \rho > 0 \). It follows from (2.9) and (2.10) that the operator \( \pi_\theta \) is the quantum analogue of a classical conditional probability. Indeed, if \( \mathcal{B}(H \otimes K) \) is replaced by commutative algebra, then \( \pi_\theta \) coincides with a classical conditional probability.

**Definition 2.4** An operator \( \pi \in \mathcal{B}(H \otimes K) \) is called the quantum conditional probability operator (QCPO, for short) if \( \pi \) satisfies condition (2.9) and (2.10).

It is easy to verify\([5]\) that for any CP unital map \( \varphi : \mathcal{B}(K) \rightarrow \mathcal{B}(H) \) and an orthonormal basis in \( K \) the following operator
\[
\pi_\varphi = \sum_{k,l=1}^{d_K} \varphi(e_{kl}) \otimes e_{kl}, \tag{2.11}
\]
defines QCPO. From Lemma 2.2 and unitality of \( \varphi \), it follows that \( \pi_\varphi \) satisfies conditions (2.9) and (2.10). For a given \( \pi_\varphi \) and any faithful marginal state \( \rho \in \mathcal{S}(H) \), one can construct a state \( \theta_\varphi \) of the composite system
\[
\theta_\varphi = \sum_{k,l=1}^{d_K} \rho^{-\frac{i}{2}} \varphi(e_{kl}) \rho^{-\frac{i}{2}} \otimes e_{kl}. \tag{2.12}
\]
It is clear that \( \theta_\varphi \) is a PPT state if and only if the map \( \varphi \) is a CCP. There exists a simple relation between the density operator \( \theta_\phi \) in (2.7) and the QCPO \( \pi_\varphi \) in (2.11) due to the following decomposition of the entanglement map \( \phi \).

**Lemma 2.5** \([12]\) Every entanglement map \( \phi \) with \( \phi(1_K) = \rho \) has a decomposition
\[
\phi(\cdot) = \rho^{-\frac{i}{2}} \varphi(\cdot) \tau(\cdot) \rho^{-\frac{i}{2}}, \tag{2.13}
\]
where \( \varphi \) is a CP unital map to be found as a unique solution to
\[
\varphi(\cdot) = \rho^{-\frac{i}{2}} \phi(\cdot) \tau(\cdot) \rho^{-\frac{i}{2}}. \tag{2.14}
\]

**Theorem 2.6** \([20]\) If a composite state \( \theta_\phi \) given by (2.7) has a faithful marginal state \( \rho = \phi(1_K) \), then \( \theta_\phi \) is represented by
\[
\theta_\phi = (\rho^{-\frac{i}{2}} \otimes 1_K) \pi_\phi (\rho^{-\frac{i}{2}} \otimes 1_K), \tag{2.15}
\]
where \( \pi_\phi = \sum_{k,l} \rho^{-\frac{i}{2}} \phi(e_{kl}) \rho^{-\frac{i}{2}} \otimes e_{kl}. \)
3 Classical and quantum information

In classical description of a physical composite system its correlation can be represented by a joint probability measure or a conditional probability measure. In classical information theory we have proper criteria to estimate such correlation, which are so-called the mutual entropy and the conditional entropy given by Shannon [42]. Here we review Shannon’s entropies briefly.

Let $X = \{x_i\}_{i=1}^{m}$ and $Y = \{y_j\}_{j=1}^{m}$ be random variables with probability distributions $p_i$ and $q_j$, respectively, and let $p_{ij}$ denotes conditional probability $P(X = x_i|Y = y_j)$. The joint probability $r_{ij} = P(X = x_i, Y = y_j)$ is given by

$$r_{ij} = p_{ij} q_j.$$  \hspace{1cm} (3.1)

Let us recall definitions of mutual entropy $I(X : Y)$ and conditional entropies $S(X \mid Y)$, $S(Y \mid X)$:

$$I(X : Y) = \sum_{i,j} r_{ij} \log \frac{r_{ij}}{p_i q_j},$$

and

$$S(X \mid Y) = -\sum_j q_j \sum_i p_{ij} \log p_{ij}, \quad S(Y \mid X) = -\sum_i p_i \sum_j p_{ij} \log p_{ij}.$$  

Using (3.1), we can easily check that the following relations

$$I(X : Y) = S(X) + S(Y) - S(XY),$$  \hspace{1cm} (3.2)

and

$$S(X \mid Y) = S(XY) - S(Y) = S(X) - I(X : Y),$$  \hspace{1cm} (3.3)

$$S(Y \mid X) = S(XY) - S(X) = S(Y) - I(X : Y),$$  \hspace{1cm} (3.4)

where $S(X) = -\sum_i p_i \log p_i$, and $S(XY) = -\sum_{i,j} r_{ij} \log r_{ij}$. Note, that $p_{ij}$ gives rise to a stochastic matrix $T_{ij} := p_{ij}$ and hence it defines a classical channel

$$p_i = \sum_j T_{ij} q_j.$$  \hspace{1cm} (3.5)

Note, that data provided by $r_{ij}$ are the same as those provided by $T_{ij}$ and $p_j$. Hence one may instead of $I(X : Y)$ use the following notation $I(P, T)$, where $P$ represent an input state and $T$ the classical channel. One interprets $I(P, T)$ as a information transmitted via a channel $T$. The fundamental Shannon inequality

$$0 \leq I(P, T) \leq \min\{S(X), S(Y)\},$$  \hspace{1cm} (3.6)

gives the obvious bounds upon the transmitted information.

Now, we extend the classical mutual entropy to the quantum system using the Umegaki relative entropy [43]. Let $\theta \in S(H \otimes K)$ with marginal states $\rho \in S(H)$ and $\sigma \in S(K)$. One defines quantum mutual entropy as a relative entropy between $\theta$ and the product of marginals $\rho \otimes \sigma$:

$$I(\theta) = S(\theta \| \rho \otimes \sigma) = \text{Tr} \{ \theta [\log \theta - \log(\rho \otimes \sigma)] \}.$$  \hspace{1cm} (3.7)

As in the classical case one shows that

$$I(\theta) = S(\rho) + S(\sigma) - S(\theta).$$  \hspace{1cm} (3.8)

Introducing quantum conditional entropy

$$S_\theta(\rho | \sigma) := S(\theta) - S(\sigma),$$  \hspace{1cm} (3.9)

one finds

$$I(\theta) = S(\rho) - S_\theta(\rho | \sigma),$$  \hspace{1cm} (3.10)

or, equivalently

$$I(\theta) = S(\sigma) - S_\theta(\sigma | \rho).$$  \hspace{1cm} (3.11)
Definition 3.1 [71, 72, 74, 22] For any entanglement map \( \phi : \mathcal{B}(\mathcal{K}) \to \mathcal{B}(\mathcal{H}) \) with \( \rho = \phi(1_\mathcal{K}) \) and \( \sigma = \phi'(1_\mathcal{H}) \), the quantum mutual entropy \( I_\theta(\rho : \sigma) \) is defined by

\[
I_\theta(\rho : \sigma) := S(\theta_\rho \| \rho \otimes \sigma) = \text{Tr} \{ \theta_\rho (\log \theta_\rho - \log(\rho \otimes \sigma)) \},
\]

where \( S(\cdot \| \cdot) \) is the Umegaki relative entropy.

One easily finds

\[
I_\theta(\rho : \sigma) = S(\rho) + S(\sigma) - S(\theta_\rho).
\]

The above relation (3.13) is a quantum analog of (3.2). One defines the quantum conditional entropies as generalizations of (3.3), (3.4) [11, 12, 14, 24]:

\[
S_\theta(\sigma | \rho) := S(\sigma) - I_\theta(\rho : \sigma) = S(\theta_\rho) - S(\rho).
\]

It is usually assumed that \( I_\theta(\rho : \sigma) \) measures all correlations encoded into the bipartite state \( \theta_\rho \) with marginals \( \rho \) and \( \sigma \).

Example 3.2 (Product state) For the entanglement map

\[
\phi(b) := \rho \text{Tr}_\mathcal{K}(\sigma b),
\]

one finds \( \theta_\rho = \rho \otimes \sigma \), and hence

\[
I_\theta(\rho : \sigma) = 0, \quad S_\theta(\sigma | \rho) = S(\sigma), \quad S_\theta(\rho | \sigma) = S(\rho),
\]

which recover well known relations for a product state \( \rho \otimes \sigma \).

Example 3.3 (Pure entangled state) Let \( \{\lambda_i\} \) be the sequence of complex numbers satisfying \( \sum_i |\lambda_i|^2 = 1 \). For entanglement mappings

\[
\phi(b) = \sum_{i,j=1}^r \lambda_i \bar{\lambda}_j e_i \langle f_j, b f_i \rangle,
\]

where \( \{e_i\} \) and \( \{f_i\} \) are orthonormal basis in \( \mathcal{H} \) and \( \mathcal{K} \), respectively, the state \( \theta_\rho \) can be written in the following form

\[
\theta_\rho = \sum_{i,j=1}^r \lambda_i \bar{\lambda}_j e_i \otimes f_j = |\Psi\rangle \langle \Psi|,
\]

where

\[
|\Psi\rangle = \sum_{i=1}^r \lambda_i e_i \otimes f_i \in \mathcal{H} \otimes \mathcal{K}.
\]

Note, that

\[
r \leq \min[d_\mathcal{H}, d_\mathcal{K}],
\]

equals to the Schmidt rank of \( \Psi \in \mathcal{H} \otimes \mathcal{K} \). One finds for the reduced states

\[
\rho = \phi(1_\mathcal{K}) = \sum_{i=1}^r |\lambda_i|^2 e_i, \quad \sigma = \phi'(1_\mathcal{H}) = \sum_{i=1}^r |\lambda_i|^2 f_i,
\]

and hence

\[
I_\theta(\rho : \sigma) = S(\rho) + S(\sigma) - S(\theta) = 2S(\rho) > \min[S(\rho), S(\sigma)],
\]

together with

\[
S_\theta(\sigma | \rho) = S_\theta(\rho | \sigma) = -S(\rho) < 0,
\]

where \( S(\rho) = S(\sigma) = -\sum_i |\lambda_i|^2 \log |\lambda_i|^2 \).
As is mentioned in Section 2, the classical mutual entropy always satisfies the Shannon’s fundamental inequality, i.e. it is always smaller than its marginal entropies, and the conditional entropy is always positive. Note that separable state has the same property. It is no longer true for pure entangled states.

Now we introduce another measure for correlation of composite states.\cite{11,12,20,34}

**Definition 3.4** For the entanglement map \( \phi : B(K) \to B(H) \), we define the D-correlation \( D(\theta) \) of \( \theta \) as

\[
D(\theta) := -\frac{1}{2} \{ S_\theta(\sigma\rho) + S_\theta(\rho\sigma) \} = \frac{1}{2}(S(\rho) + S(\sigma)) - S(\theta) .
\] (3.18)

Note that the D-correlation with the opposite convention \(-D(\theta)\) is called the degree of entanglement.\cite{11,12,20,34} One proves the following:

**Proposition 3.5**\cite{2,34} If \( \theta_0 \) is a pure state, then the following statements hold:

1. \( \theta \) is entangled state if and only if \( D(\theta) > 0 \).
2. \( \theta \) is separable state if and only if \( D(\theta) = 0 \).

It is well-known that if \( \theta \) is a PPT state, then

\[
S(\theta) - S(\rho) \geq 0, \quad S(\theta) - S(\sigma) \geq 0,
\] (3.19)

where \( \rho \) and \( \sigma \) are the marginal states of \( \theta \).\cite{44}

**Proposition 3.6** If \( \theta \) is a PPT state, then

\[
D(\theta) \leq 0. \quad (3.20)
\]

Suppose now that we have two entanglement mappings \( \phi_k : B(K) \to B(H) \), \((k = 1, 2)\) such that \( \phi_1(1_K) = \phi_2(1_K) \) and \( \phi'_1(1_H) = \phi'_2(1_H) \). Let \( \theta_1, \theta_2 \in S(H \otimes K) \) be the corresponding states. We propose the following:

**Definition 3.7** \( \theta_1 \) is said to have stronger D-correlations than \( \theta_2 \) if

\[
D(\theta_1) > D(\theta_2) . \quad (3.21)
\]

Several measures of correlation based on entropic quantities were already discussed by Cerf and Adami\cite{14}, Horodecki\cite{24}, Henderson and Vedral\cite{23}, Groisman et al.\cite{22}.

### 4 Quantum discord

Let us briefly recall the definition of quantum discord \cite{39,23}. Recall, that mutual information may be rewritten as follows

\[
I(\theta) = S(\sigma) - S_\theta(\sigma|\rho) . \quad (4.1)
\]

An alternative way to compute the conditional entropy \( S_\theta(\sigma|\rho) \) goes as follows: one introduces a measurement on \( H \)-party defined by the collection of one-dimensional projectors \( \{ \Pi_k \} \) in \( H \) satisfying \( \Pi_1 + \Pi_2 + \ldots = 1_H \). The label ‘\( k \)’ distinguishes different outcomes of this measurement. The state after the measurement when the outcome corresponding to \( \Pi_k \) has been detected is given by

\[
\theta_{k|k} = \frac{1}{p_k} (\Pi_k \otimes 1_K) \theta (\Pi_k \otimes 1_K) , \quad (4.2)
\]

where \( p_k \) is a probability that \( H \)-party observes \( k \)th result, i.e. \( p_k = \text{Tr}(\Pi_k \rho) \), and \( \theta_{k|k} \) is the (collapsed) state in \( H \otimes K \), after \( H \)-party has observed \( k \)th result in her measurement. The entropies \( S(\theta_{k|k}) \) weighted by probabilities \( p_k \) yield the conditional entropy of part \( K \) given the complete measurement \( \{ \Pi_k \} \) on the part \( H \)

\[
S(\theta|\{ \Pi_k \}) = \sum_k p_k S(\theta_{k|k}) . \quad (4.3)
\]

Finally, let

\[
I(\theta|\{ \Pi_k \}) = S(\sigma) - S(\theta|\{ \Pi_k \}) , \quad (4.4)
\]
be the corresponding measurement induced mutual information. The quantity
\[
C_H(\theta) = \sup_{[\Pi_0]} \mathcal{I}(\theta | \Pi_0),
\]
(4.5)
is interpreted [23, 21] as a measure of classical correlations. Now, these two quantities – \( \mathcal{I}(\theta) \) and \( C_H(\theta) \) – may differ and the difference
\[
\mathcal{D}_H(\theta) = \mathcal{I}(\theta) - C_H(\theta)
\]
is called a quantum discord.

Evidently, the above definition is not symmetric with respect to parties \( \mathcal{H} \) and \( \mathcal{K} \). However, one can easily swap the role of \( \mathcal{H} \) and \( \mathcal{K} \) to get
\[
\mathcal{D}_K(\theta) = \mathcal{I}(\theta) - C_K(\theta),
\]
(4.7)
where
\[
C_K(\theta) = \sup_{[\Pi_0]} \mathcal{I}(\theta | \Pi_0),
\]
(4.8)
and \( \Pi_0 \) is a collection of one-dimensional projectors in \( \mathcal{K} \) satisfying \( \Pi_1 + \Pi_2 + \ldots = 1_\mathcal{K} \). For a general mixed state \( \mathcal{D}_H(\theta) \neq \mathcal{D}_K(\theta) \). However, it turns out that \( \mathcal{D}_H(\theta), \mathcal{D}_K(\theta) \geq 0 \). Moreover, on pure states, quantum discord coincides with the von Neumann entropy of entanglement \( S(\rho) = S(\sigma) \). States with zero quantum discord – so called classical-quantum states – represent essentially a classical probability distribution \( p_k \) embedded in a quantum system. One shows that \( \mathcal{D}_H(\theta) = 0 \) if and only if there exists an orthonormal basis \( |k\rangle \) in \( \mathcal{H} \) such that
\[
\theta = \sum_k p_k |k\rangle \langle k| \otimes \sigma_k,
\]
(4.9)
where \( \sigma_k \) are density matrices in \( \mathcal{K} \). Similarly, \( \mathcal{D}_K(\theta) = 0 \) if and only if there exists an orthonormal basis \( |\alpha\rangle \) in \( \mathcal{K} \) such that
\[
\theta = \sum_\alpha q_\alpha \rho_\alpha \otimes |\alpha\rangle \langle \alpha|,
\]
(4.10)
where \( \rho_\alpha \) are density matrices in \( \mathcal{H} \). It is clear that if \( \mathcal{D}_H(\theta) = \mathcal{D}_K(\theta) = 0 \), then \( \theta \) is diagonal in the product basis \( |k\rangle \otimes |\alpha\rangle \) and hence
\[
\theta = \sum_{k,\alpha} \lambda_{ka} |k\rangle \langle k| \otimes |\alpha\rangle \langle \alpha|,
\]
(4.11)
is fully encoded by the classical joint probability distribution \( \lambda_{ka} \).

Finally, let us introduce a symmetrized quantum discord
\[
\mathcal{D}_{H,K}(\theta) := \frac{1}{2} \left[ \mathcal{D}_H(\theta) + \mathcal{D}_K(\theta) \right].
\]
(4.12)
Let us observe that there is an intriguing relation between (4.12) and (3.13). One has
\[
\mathcal{D}(\theta) = \mathcal{I}(\theta) - \frac{1}{2} [S(\rho) + S(\sigma)],
\]
(4.13)
whereas
\[
\mathcal{D}_{H,K}(\theta) = I(\theta) - C_{H,K}(\theta).
\]
(4.14)
Note, that \( \mathcal{D}_{H,K}(\theta) \geq 0 \) but \( \mathcal{D}(\theta) \) can be negative (for PPT states). It is assumed that \( \mathcal{D}_{H,K}(\theta) \) measures perfectly quantum correlations encoded into \( \theta \).

**Example 4.1 (Separable correlated state)** For the entanglement map given by
\[
\phi(b) = \sum_i \lambda_i \rho_i \text{Tr}_b b, \quad \phi^* (a) = \sum_i \lambda_i \sigma_i \text{Tr}_a a, \quad \left( \sum_i \lambda_i = 1, \lambda_i \geq 0 \forall i \right).
\]
the corresponding state \( \theta \) can be written in the form
\[
\theta = \sum_i \lambda_i \rho_i \otimes \sigma_i,
\]
(4.15)
with \( \rho = \phi(1_\mathcal{K}) = \sum_i \lambda_i \rho_i \) and \( \sigma = \phi^*(1_\mathcal{H}) = \sum_i \lambda_i \sigma_i \). Then, we have the following inequalities. [3, 7, 22]
\[
S(\rho) \geq 0, \quad S(\rho | \sigma) \geq 0.
\]
(4.16, 4.17)
Example 4.2 (Separable perfectly correlated state) Let \( \{e_i\} \) and \( \{f_j\} \) be the complete orthonormal systems in \( \mathcal{H} \) and \( \mathcal{K} \), respectively. For the entanglement map given by

\[
\phi(b) = \sum_i \lambda_i |e_i\rangle\langle f_i| b|e_i\rangle,
\]

the corresponding state \( \theta \) can be written in the form

\[
\theta = \sum_i \lambda_i |e_i\rangle\langle f_i|,
\]

with \( \rho = \phi(1_\mathcal{K}) = \sum_i \lambda_i |e_i\rangle\langle e_i| \), \( \sigma = \phi^* (1_\mathcal{H}) = \sum_i \lambda_i |f_i\rangle\langle f_i| \). It is clear that \( D_{\mathcal{H},\mathcal{K}}(\theta) = 0 \). Moreover, one obtains

\begin{align}
I(\theta) &= S(\rho) + S(\sigma) - S(\theta_{\rho}) = S(\rho), \\
S_{\rho}(\sigma|\rho) &= S_{\rho}(\rho|\sigma) = 0,
\end{align}

(4.18) (4.19)

where \( S(\rho) = S(\sigma) = S(\theta_{\rho}) = -\sum_i \lambda_i \log \lambda_i \). This correlation corresponds to a perfect correlation in the classical scheme.

5 Quantum correlations for circulant states

In this section, we analyze correlations encoded into the special family of so called circulant states.

5.1 A circulant state

We start this section by recalling the definition of a circulant state introduced in \([17]\) (see also \([18]\)). Consider the finite dimensional Hilbert space \( \mathbb{C}^d \) with the standard basis \( \{e_0, e_1, \ldots, e_{d-1}\} \). Let \( \Sigma_0 \) be the subspace of \( \mathbb{C}^d \otimes \mathbb{C}^d \) generated by \( e_i \otimes e_i \) \( (i = 0, 1, \ldots, d - 1) \):

\[
\Sigma_0 = \text{span} \{ e_0 \otimes e_0, e_1 \otimes e_1, \ldots, e_{d-1} \otimes e_{d-1} \}.
\]

(5.1)

Define a shift operator \( S^a : \mathbb{C}^d \rightarrow \mathbb{C}^d \) by

\[
S^a e_k = e_{k+a} \mod d,
\]

and let

\[
\Sigma_a := (1_d \otimes S^a) \Sigma_0.
\]

(5.2)

It turns out that \( \Sigma_a \) and \( \Sigma_\beta \) \( (a \neq \beta) \) are mutually orthogonal and one has the following direct sum decomposition

\[
\mathbb{C}^d \otimes \mathbb{C}^d \cong \Sigma_0 \oplus \Sigma_1 \oplus \cdots \oplus \Sigma_{d-1}.
\]

(5.3)

This decomposition is called a circulant decomposition.\([17]\) Let \( a^{(0)}, a^{(1)}, \ldots, a^{(d-1)} \) be positive \( d \times d \) matrices with entries in \( \mathbb{C} \) such that \( \rho_\alpha \) is supported on \( \Sigma_a \). Moreover, let

\[
\text{tr}(a^{(0)} + \cdots + a^{(d-1)}) = 1.
\]

(5.4)

Now, for each \( a^{(\alpha)} \in M_d(\mathbb{C}) \) one defines a positive operator in \( \mathbb{C}^d \otimes \mathbb{C}^d \) be the following formula

\[
\theta_\alpha = \sum_{i,j=0}^{d-1} a^{(\alpha)}_{ij} e_i \otimes S^a e_j S^{a\dagger}.
\]

(5.5)

Finally, let us introduce

\[
\theta := \theta_0 \oplus \cdots \oplus \theta_{d-1}.
\]

(5.6)

One proves\([17]\) that \( \rho \) defines a legitimate density operators in \( \mathbb{C}^d \otimes \mathbb{C}^d \). One calls it a circulant state. For further details of circulant states we refer to Refs. \([17, 18]\).

Now, let consider a partial transposition of the circulant state. It turns out that \( \rho^{\tau} = (1 \otimes \tau) \rho \) is again circulant but it corresponds to another cyclic decomposition of the original Hilbert space \( \mathbb{C}^d \otimes \mathbb{C}^d \). Let us
introduce the following permutation \( \pi \) from the symmetric group \( S_d \): it permutes elements \( \{0, 1, \ldots, d-1\} \) as follows
\[
\pi(0) = 0, \quad \pi(i) = d - i, \quad i = 1, 2, \ldots, d-1. \tag{5.7}
\]
We use \( \pi \) to introduce
\[
\Sigma_0 = \text{span} \{ e_0 \otimes e_{\pi(0)}, e_1 \otimes e_{\pi(1)}, \ldots, e_{d-1} \otimes e_{\pi(d-1)} \}, \tag{5.8}
\]
and
\[
\tilde{\Sigma}_0 = (I \otimes S^0) \Sigma_0. \tag{5.9}
\]
It is clear that \( \tilde{\Sigma}_0 \) and \( \tilde{\Sigma}_\beta \) are mutually orthogonal (for \( \alpha \neq \beta \)). Moreover,
\[
\tilde{\Sigma}_0 \oplus \cdots \oplus \tilde{\Sigma}_{d-1} = C^d \otimes C^d, \tag{5.10}
\]
and hence it defines another circulant decomposition. Now, the partially transformed state \( \vartheta^s \) has again a circulant structure but with respect to the new decomposition (5.10):
\[
\vartheta^s = \vartheta^{(0)} + \cdots + \vartheta^{(d-1)}, \tag{5.11}
\]
where
\[
\vartheta^{(\alpha)} = \sum_{i,j=0}^{d-1} \vartheta_{ij}^{(\alpha)} e_{ij} \otimes S^\alpha e_{\pi(i)\pi(j)} S^{\dagger \alpha}, \quad \alpha = 0, \ldots, d-1. \tag{5.12}
\]
and the new \( d \times d \) matrices \( \vartheta_{ij}^{(\alpha)} \) are given by the following formulae:
\[
\tilde{\alpha}^{(\alpha)} = \sum_{\beta=0}^{d-1} a^{(\alpha+\beta)} \circ (\Pi S^\beta), \quad \text{mod } d, \tag{5.13}
\]
where “\( \circ \)” denotes the Hadamard product and \( \Pi \) being a \( d \times d \) permutation matrix corresponding to \( \pi \), i.e. \( \Pi_{ij} := \delta_{\pi(i),j} \). It is therefore clear that our original circulant state is PPT iff all \( d \) matrices \( \vartheta^{(\alpha)} \) satisfy
\[
\tilde{\alpha}^{(\alpha)} \geq 0, \quad \alpha = 0, \ldots, d-1. \tag{5.14}
\]

### 5.2 Generalized Bell diagonal states

The most important example of circulant states is provided by Bell diagonal states [6, 7, 8] defined by
\[
\rho = \sum_{m,n=0}^{d-1} P_{mn} P_{mn}, \tag{5.15}
\]
where \( p_{mn} \geq 0, \sum_{m,n} p_{mn} = 1 \) and
\[
P_{mn} = (I \otimes U_{mn}) P_d (I \otimes U_{mn}^\dagger), \tag{5.16}
\]
with \( U_{mn} \) being the collection of \( d^2 \) unitary matrices defined as follows
\[
U_{mn} e_k = \lambda^{mk} S^\alpha e_k = \lambda^{mk} e_{k+n}, \tag{5.17}
\]
with
\[
\lambda = e^{2\pi i/d}. \tag{5.18}
\]
The matrices \( U_{mn} \) define an orthonormal basis in the space \( M_d(\mathbb{C}) \) of complex \( d \times d \) matrices. One easily shows
\[
\text{Tr}(U_{mn} U_{nm}^\dagger) = d \delta_{mr} \delta_{ns}. \tag{5.19}
\]
Some authors call \( U_{mn} \) generalized spin matrices since for \( d = 2 \) they reproduce standard Pauli matrices:
\[
U_{00} = I, \quad U_{01} = \sigma_1, \quad U_{10} = i\sigma_2, \quad U_{11} = \sigma_3. \tag{5.20}
\]
Let us observe that Bell diagonal states (5.15) are circulant states in \( \mathbb{C}^d \otimes \mathbb{C}^d \). Indeed, maximally entangled projectors \( P_{mn} \) are supported on \( \Sigma_n \), that is,

\[
\Pi_n = P_{0n} + \ldots + P_{dn-1,n},
\]

defines a projector onto \( \Sigma_n \), i.e.

\[
\Sigma_n = \Pi_n (\mathbb{C}^d \otimes \mathbb{C}^d).
\]

One easily shows that the corresponding matrices \( \delta^{(n)} \) are given by

\[
da^{(n)} = HD^{(n)}H^*,
\]

where \( H \) is a unitary \( d \times d \) matrix defined by

\[
H_{kl} := \frac{1}{\sqrt{d}} \delta^{kl},
\]

and \( D^{(n)} \) is a collection of diagonal matrices defined by

\[
D_{kl}^{(n)} := p_{nn} \delta_{kl}.
\]

One has

\[
da^{(n)}_{kl} = \frac{1}{d} \sum_{m=0}^{d-1} p_{nm} \lambda_m^{(k-l)},
\]

and hence it defines a circulant matrix

\[
da^{(n)}_{kl} = f^{(n)}_{k-l},
\]

where the vector \( f^{(n)}_{m} \) is the inverse of the discrete Fourier transform of \( p_{nn} \) (\( n \) is fixed).

### 5.3 A family of Horodecki states

Let \( \mathcal{H} = \mathcal{K} = \mathbb{C}^3 \). For any \( \alpha \in [0,5] \), one defines\(^{26}\) the following state

\[
\theta_1(\alpha) = \frac{2}{7} P_3^* + \frac{\alpha}{7} \Pi_1 + \frac{5-\alpha}{7} \Pi_2.
\]

The eigenvalues of \( \theta_1(\alpha) \) are calculated as 0, \( \frac{2}{7} \), \( 3 \times \frac{3}{21} \) and \( 3 \times \frac{5-\alpha}{21} \) and hence one obtains for the \( D \)-correlations

\[
D(\theta_1(\alpha)) = \log 3 + \frac{2}{7} \log \frac{2}{7} + \frac{\alpha}{7} \log \frac{\alpha}{21} + \frac{5-\alpha}{7} \log \frac{5-\alpha}{21}.
\]

**Theorem 5.1**\(^{26}\) The family \( \theta_1(\alpha) \) satisfies:

1. \( \theta_1(\alpha) \) is PPT if and only \( \alpha \in [1,4] \)
2. \( \theta_1(\alpha) \) is separable if and only \( \alpha \in [2,3] \);
3. \( \theta_1(\alpha) \) is both entangled and PPT if and only \( \alpha \in [1,2] \cup (3,5] \);
4. \( \theta_1(\alpha) \) is NPT if and only \( \alpha \in [0,1] \cup (4,5] \).

Due to this Theorem, one can find that the \( D(\theta_1(\alpha)) \) does admit a natural order. That is, the \( D \)-correlation for any entangled state is always stronger than \( D \)-correlation for an arbitrary separable state. Similarly, one observes that \( D \)-correlation for any NPT state is always stronger than \( D \)-correlation for an arbitrary PPT state. The graph of \( D(\theta_1(\alpha)) \) is shown in Fig.2. Actually, one finds that the minimal value of \( D \)-correlations corresponds to \( \alpha = 2.5 \), that is, it lies in the middle of the separable region.

On the other hand, we can also compute the symmetrized discord \( \mathcal{D}_{\mathbb{C}^1 \otimes \mathbb{C}^1}(\theta_1(\alpha)) \) and have obtained Fig.2. It is easy to find that the graph is symmetric with respect to \( \alpha = 2.5 \). As in Fig. 2, the value of the symmetrized discord satisfies the following inequality:

\[
0 < \mathcal{D}_{\mathbb{C}^1 \otimes \mathbb{C}^1}(\theta_1(\alpha)) \leq \mathcal{D}_{\mathbb{C}^1 \otimes \mathbb{C}^1}(\theta_1(\beta)) \leq \mathcal{D}_{\mathbb{C}^1 \otimes \mathbb{C}^1}(\theta_1(\gamma)),
\]
where $\alpha \in [2, 3]$, $\beta \in [1, 2] \cup [3, 4]$ and $\gamma \in [0, 1] \cup [4, 5]$.

The family of $\theta_1(\alpha)$ has the quantum correlation even in separable states corresponding to $\alpha \in [2, 3]$ in the sense of discord. We know that the above two types of criteria give the similar order of correlation.

Notice that $D(\theta_1(\alpha))$ is always negative even in NPT states and the positivity of $D$-correlation represents a true quantum property (see Example 3.3 and Proposition 3.5). In this sense the quantum correlation of $\theta_1(\alpha)$ is not so strong.

This family may be generalized to $\mathbb{C}^d \otimes \mathbb{C}^d$ as follows: consider the following family of circular 2-qudit states

$$
\theta(\alpha) = \sum_{i=1}^{d-1} \lambda_i \Pi_i + \lambda_d P_d^r,
$$

with $\lambda_i \geq 0$, and $\lambda_1 + \ldots + \lambda_{d-1} + \lambda_d = 1$. Let us take the following special case corresponding to

$$
\lambda_1 = \frac{\alpha}{\ell}, \quad \lambda_{d-1} = \frac{(d-1)^2 + 1 - \alpha}{\ell}, \quad \lambda_d = \frac{d-1}{\ell}.
$$

and $\lambda_2 = \ldots = \lambda_{d-2} = \lambda_d$, with

$$
\ell = (d-1)(2d-3) + 1.
$$

One may prove the following[21]

**Theorem 5.2** The family $\theta(\alpha)$ satisfies:

1. $\theta(\alpha)$ is PPT if and only $\alpha \in [1, (d-1)^2]$
2. $\theta(\alpha)$ is separable if and only if $\alpha \in [d-1, (d-1)(d-2) + 1]$;
3. $\theta(\alpha)$ is both entangled and PPT if and only if $\alpha \in [1, d-1) \cup ((d-1)(d-2) + 1, (d-1)^2]$;
4. $\theta(\alpha)$ is NPT if and only if $\alpha \in [0, 1) \cup ((d-1)^2, (d-1)^2 + 1]$.

For example if $d = 4$ one obtains the following picture of $D(\theta(\alpha))$ (see Fig. 4) Again, one finds that

$$
D(\theta(\alpha)) \text{ does admit a natural order. That is, the } D\text{-correlation for any entangled state is always stronger than } D\text{-correlation for an arbitrary separable state. Similarly, one observes that } D\text{-correlation for any NPT state is always stronger than } D\text{-correlation for an arbitrary PPT state.}$$
5.4 Example: a family of Bell diagonal states

Consider the following class of Bell-diagonal states in $\mathbb{C}^3 \otimes \mathbb{C}^3$:

$$\theta_2(\varepsilon) = \frac{1}{\Lambda} (3P^*_3 + \varepsilon \Pi_1 + \varepsilon^{-1} \Pi_2),$$

with $\Lambda = 1 + \varepsilon + \varepsilon^{-1}$. One easily finds for its $D$-correlations

$$D(\theta_2(\varepsilon)) = \frac{1}{\Lambda} \left( \log \frac{1}{\Lambda} + \varepsilon^{-1} \log \frac{\varepsilon^{-1}}{\Lambda} + \varepsilon \log \frac{\varepsilon}{\Lambda} + \log 3 \right).$$

(5.34)

The following theorem gives us a useful characterization of $\theta_2(\varepsilon)$ [30].

**Theorem 5.3** The states of $\theta_1(\varepsilon)$ are classified by $\varepsilon$ as follows:

1. $\theta_2(\varepsilon)$ is separable if $\varepsilon = 1$;

2. $\theta_2(\varepsilon)$ is both PPT and entangled for $\varepsilon \neq 1$.

The graph of $D(\theta_2(\varepsilon))$ is shown in Fig. 2. $D(\theta_2(\varepsilon))$ is rapidly decreasing with $\varepsilon$ approaching 1 from 0 and increases when $\varepsilon$ is over 1. That is, $D(\theta_2(\varepsilon))$ takes the minimal value at $\varepsilon = 1$ and it is approximated about $D(\theta_2(1)) = -\frac{3}{4} \log 3 \approx -0.7324$. As is the case of $\theta_1(\varepsilon)$, the $D$-correlation $D(\theta_2(\varepsilon))$ for an entangled state is always stronger than the one for a separable state. As $\varepsilon \to 0$ or $\infty$, $\theta_2(\varepsilon)$ converges to a separable perfectly correlated state which can be recognized as a “classical state”

$$\lim_{\varepsilon \to 0} \theta_2(\varepsilon) = \frac{1}{3} (e_{00} \otimes e_{11} + e_{11} \otimes e_{00} + e_{22} \otimes e_{11}) = \Pi_2,$$

(5.35)

and for every $\varepsilon > 0$,

$$D(\theta_2(\varepsilon)) < 0 = \lim_{\varepsilon \to 0} D(\theta_2(\varepsilon)) = \lim_{\varepsilon \to \infty} D(\theta_2(\varepsilon)).$$

(5.37)

It shows that a correlation of a PPT entangled state $\theta_2(\varepsilon \neq 1)$ is weaker than that of the (classical) separable perfectly correlated states in the sense of (3.21).

Now, since $\theta_1(\varepsilon)$ and $\theta_2(\varepsilon)$ have common marginal states, we can compare the order of quantum correlations for them. One has, for example,

$$D(\theta_2(1)) \approx -0.7324 > -0.7587 \approx D(\theta_1(3.1)).$$

(5.38)

Accordingly Theorem 5.1 and 5.3 however, $\theta_2(1)$ is separable while $\theta_1(3.1)$ is entangled state. Incidentally, this means that the correlation for the separable state $\theta_2(1)$ is stronger than the entangled state $\theta_1(3.1)$ in the sense of (3.21).

---

**Figure 3:** Left — the graph of $D(\theta_2(x))$. Note that $D$ is minimal for $x = 1$ which correspond to the separable state. Right — the graph of $D(\mathbb{C}^3 \otimes \mathbb{C}^3)(\theta_2(\varepsilon))$ for $\varepsilon \in (0, 1]$. Note that $D(\mathbb{C}^3 \otimes \mathbb{C}^3)(\theta_2(\varepsilon)) = D(\mathbb{C}^3 \otimes \mathbb{C}^3)(\theta_2(\varepsilon^{-1}))$.

On the other hand one finds the following plot of the quantum discord Fig. 3. It is clear that

$$\lim_{\varepsilon \to 0} D(\mathbb{C}^3 \otimes \mathbb{C}^3)(\theta_2(\varepsilon)) = \lim_{\varepsilon \to \infty} D(\mathbb{C}^3 \otimes \mathbb{C}^3)(\theta_2(\varepsilon)) = 0,$$

(5.39)

since both $\Pi_1$ and $\Pi_2$ are perfectly classical states. Note, that $D(\mathbb{C}^3 \otimes \mathbb{C}^3)(\theta_2(\varepsilon = 1)) > 0$ which shows that separable state $\theta_2(\varepsilon = 1)$ does contain quantum correlations.
6 Conclusions

We provided several examples of bi-partite quantum states and computed two types of correlations for them. It turned out that the correlation for a separable state can be stronger than the one for an entangled state in the sense of (3.21). This observation is inconsistent with the conventional understanding of quantum entanglement. However, we also showed that the discord of such separable states might strictly positive. This means that these states have a non-classical correlation. From this point of view, it is no longer unusual that the correlation for a separable state is stronger than the one for an entangled state.

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