Optimal measurements to access classical correlations of two-qubit states

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We analyze the optimal measurements accessing classical correlations in arbitrary two-qubit states. Two-qubit states can be transformed into the canonical forms via local unitary operations. For the canonical forms, we investigate the probability distribution of the optimal measurements. The probability distribution of the optimal measurement is found to be centralized in the vicinity of a specific von Neumann measurement, which we call the maximal-correlation-direction measurement (MCDM). We prove that for the states with zero-discord and maximally mixed marginals, the MCDM is the very optimal measurement. Furthermore, we give an upper bound of quantum discord based on the MCDM, and investigate its performance for approximating the quantum discord.

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I. INTRODUCTION

Optimization procedures are involved in many quantities in the quantum information theory. One of the most important examples is the entanglement of formation, which is defined as the least expected entanglement over all ensembles of pure states realizing the given states [1]. Here we focus on the optimization procedure involved in the classical correlation, which is defined as the maximal amount of information about the subsystem B that can be obtained via performing measurement on the other subsystem A [2]. Meanwhile, the non-classical correlation is measured by the so-called quantum discord [3], which is the difference of the total amount of correlations and the classical correlation. Over the past decade, quantum discord has received a lot of attention, including analytic calculations for some special two-qubit states [4, 5], detecting of quantum discord [6–13], quantum discord in the concrete physical models [14–22], the dynamics of quantum discord [23–32], quantum discord in continuous variable system [33–37], quantum discord of multipartite states [38], and exploration in the laboratory [39–41], etc. Most recently, operational interpretations of quantum discord are proposed in Ref. [42, 43], where quantum discord was shown to be a quantitative measure about the performance in the quantum state merging.

To access the total classical correlation or get the value of quantum discord, one has to find the corresponding optimal measurements. On the other hand, the sudden change of the optimal measurements during evolution is related to a novel phenomenon of the quantum discord—the sudden change in decay rates [27–30, 40]. So a study on the optimal measurements will help us to understand the dynamical properties of the quantum discord. The optimization involved is taken over general measurements, which is described by a positive-operator-valued measure (POVM). In Ref. [44], Hamieh et al. showed that for two-qubit system the optimal measurement over POVM is a projective measurement. In this paper, we only consider orthogonal projective measurements, known as von Neumann measurement. Despite recent progress, the optimization procedure over von Neumann measurements is still hard to be resolved for general two-qubit states, and analytic approaches still lack. This motivates us to systematically investigate the optimal measurements and find an effective way to approach the optimal measurement.

In the present article, we investigate the probability distribution of the optimal measurements. Based on a general analysis on those factors which influence the classical correlation, we introduce the canonical forms for the two-qubit states and the maximal-correlation-direction measurement (MCDM). For arbitrary two-qubit states, the optimal measurements are found to be centralized in the vicinity of the MCDM. We prove that for the states with zero-discord and maximally mixed marginal, the MCDM is the very optimal measurement accessing classical correlation. We also study its veracity for X-states and arbitrary states. Then we propose the MCDM-based discord as an upper bound of quantum discord. It is demonstrated that the MCDM-based could be a good approximation of quantum discord.

This article is organized as follows. In Sec. II we give a brief review on the measures of the total, quantum and classical correlations. In Sec. III first we give a general analysis on those factors which influence the classical correlations. Then we introduced the concepts of the canonical form and the MCDM. In Sec. IV we investigate the probability distribution of the optimal measurements and the performance of the MCDM. In Sec. V we propose the MCDM-based discord as an upper bound of quantum discord, and investigate its performance for approximating quantum discord. Section VI is the conclusion.

II. REVIEW OF QUANTUM DISCORD

First, we recall the concepts of the total amount of correlations, the classical correlation and the quantum correlation. Given a quantum state $\rho$ in a composite Hilbert space $H = H^A \otimes H^B$, the total amount of correlation is...
quantified by the quantum mutual information $I$:

$$I(\rho) = S(\rho^a) + S(\rho^b) - S(\rho),$$

where $S(\rho) \equiv -\text{Tr}[\rho \log_2 \rho]$ is the von Neumann entropy and $\rho^A(B) = \text{Tr}_{B(A)}[\rho]$ is the reduced density matrix by tracing out system $B(A)$. The total amount of correlations can be split into the quantum and the classical parts.

The classical correlation is seen as the amount of information about the subsystem $B$ that can be obtained via performing a measurement on the other subsystem $A$. Then the measure of the classical correlation is defined by

$$C(\rho) = S(\rho^B) - \min_{\{E^A_k\}} \sum_k p_k S(\rho^B_k),$$

where $\{E^A_k\}$ is the POVM performed on $A$ and $\rho^B_k := \text{Tr}_A (E^A_k \otimes 1^B_\rho) / p_k$ is the remaining state of $B$ after obtaining the outcome $k$ on $A$ with the probability $p_k := \text{Tr}(E^A_k \otimes 1^B_\rho)$. $1^A(B)$ is the identity operator on the subsystem $A(B)$. Meanwhile, the quantum correlation is measured via the quantum discord defined by

$$D(\rho) = I(\rho) - C(\rho),$$

which is the difference of the total amount of correlation $I(\rho)$ and the classical correlation $C(\rho)$.

The definition of the classical and quantum correlations involves an optimization process to minimize the term $\sum_k p_k S(\rho^B_k)$, which is considered as the quantum version of the conditional entropy $\max$.

For two-qubit systems, it is shown that the optimal POVM is a projective measurement. Hereafter, we will only consider the orthogonal measurement projective measurement, known as von Neumann measurement. A von Neumann measurement $\{\Pi^A_1, \Pi^A_2\}$ of a two-qubit system can be characterized by a unit vector $n = (n_1, n_2, n_3)^T$ on the Bloch sphere, through

$$\Pi^A_1 = \frac{1}{2} \left( 1^A + \sum_{i=1}^3 n_i \sigma^A_i \right),$$

$$\Pi^A_2 = \frac{1}{2} \left( 1^A - \sum_{i=1}^3 n_i \sigma^A_i \right).$$

So the optimization may be taken over half of the Bloch sphere, since exchanging $\Pi^A_1$ and $\Pi^A_2$ gives the same measurement.

### III. General Analysis and Maximal-Correlation-Direction Measurement

The classical correlation can be expressed as

$$C = \max_{\{\Pi^A_k\}} \sum_k p_k S(\rho^B_k | \rho^B),$$

where $S(\rho^B_k | \rho^B) := -S(\rho^B_k) - \text{Tr}(\rho^B_k \log_2 \rho^B)$ is the relative entropy. If we consider the relative entropy as a measure of the distance, then the classical correlation can be considered as maximal average distance between the remaining state $\rho^B_k$ and the reduced state $\rho^B$. It seems that the optimal measurement tends to be the one which makes the remaining states far away from the reduced state, although the probability $p_k$ also plays an important role in the actual optimization problem.

Based on this tendency, we use the following Fano-Bloch decomposition of an arbitrary two-qubit state:

$$\rho = \rho^A \otimes \rho^B + \frac{1}{4} \sum_{ij=1}^3 \Lambda_{ij} \sigma^A_i \otimes \sigma^B_j,$$

where $\Lambda_{ij} = \langle \sigma^A_i \sigma^B_j \rangle_{\rho} - \langle \sigma^A_i \rangle_{\rho} \langle \sigma^B_j \rangle_{\rho}$ is the correlation function with $\langle O \rangle_{\rho} := \text{Tr}[O \rho]$ defined. This form was used to investigate the dynamics of open quantum systems in the presence of initial correlation, and the correlation functions were used to characterize the correlations in a quantum state of a composite system. Because the quantum and classical correlations are both invariant under local unitary transformations, we will consider a special set of two-qubit states, in which for arbitrary two-qubit state we can find an equivalent state up to local unitary transformations. In Ref. [4], Luo showed that the matrix $\Lambda$ in Eq. (5) can be diagonalized through local unitary transformations. Furthermore, the order and the signs of the eigenvalues of $\Lambda$ can be realigned through local unitary transformations. So studying the states in the canonical form up to local unitary transformations. Here we introduce the canonical form of two-qubit states, which is defined by

$$\rho = \rho^A \otimes \rho^B + \frac{1}{4} \sum_{i=1}^3 \Lambda_i \sigma^A_i \otimes \sigma^B_i,$$

with $\Lambda_i = \langle \sigma^A_i \sigma^B_1 \rangle_{\rho} - \langle \sigma^A_i \rangle_{\rho} \langle \sigma^B_1 \rangle_{\rho}$ and $\Lambda_1 \geq \Lambda_2 \geq |\Lambda_3|$. The sign of $\Lambda_3$ is determined by the determinant $|\Lambda|$ via $|\Lambda| = \Lambda_1 \Lambda_2 \Lambda_3$. An arbitrary two-qubit state is equivalent to a certain state in the canonical form up to local unitary transformations. So studying the states in the canonical form is adequate to understand the quantum and classical correlations of arbitrary two-qubit states. Hence, we will only consider the states in the canonical form hereafter.

After von Neumann measurement characterized by Eq. (5) performed on $A$, we get the remaining state of $B$ with the outcome $k = 1, 2$ on $A$ as follows

$$\rho^B_k = \rho^B + \frac{1}{p_k} \Delta_k,$$

where $p_k = \text{Tr}[\rho^A \Pi^A_k]$ and $\Delta_k \equiv \frac{1}{2} (-1)^{k+1} \sum_{i=1}^3 n_i \Lambda_i \sigma^B_i$ are both dependent on $\Pi^A_k(n_i)$. Note that $\Delta_2 = -\Delta_1$. From Eq. (7), we can see that the von Neumann measurement influences the quantum
conditional entropy through $p_k$ and $\Delta_k$. The influence of $p_k$ is complicated, since $p_k$ not only impacts the remaining state $\rho_k^B$ but also impacts the averaging of $S(\rho_k^B)$, while $\Delta_k$ only impacts the remaining state. If we assume that the influence of $\Delta_k$ to the quantum conditional entropy is stronger than that of $p_k$, the optimal measurement will tend to be the one which maximizes $|\Delta_1| = \sqrt{\text{Tr} \Delta_1 |\Delta_1|^T}$. (Remind $|\Delta_2| = |\Delta_1|$.)

After some algebras, we have

$$|\Delta_1|^2 = \frac{1}{16} \sum_{i=1}^3 \Lambda_i^2 n_i^2 \leq \frac{1}{16} \Lambda^2_1.$$  

(8)

The maximum of $|\Delta_1|^2$ is achieved when $n = (1, 0, 0)^T$. So the corresponding measurement is

$$\left\{ \Pi_{1}^A = \frac{1}{2}(1 + \sigma_{1}^{A}), \Pi_{2}^A = \frac{1}{2}(1 - \sigma_{1}^{A}) \right\}.$$  

(9)

Because $\Lambda_{1}$ are correlation functions and $\Lambda_{1}$ is the largest one of them, we call Eq. (9) the maximal-correlation-direction measurement (MCDM) performed on $A$ for the two-qubit states in the canonical form. For an arbitrary two-qubit state, we can always find a local unitary transformation $U_{1} \otimes U_{2}$ such that $\hat{\rho} = U_{1} \otimes U_{2} \rho U_{1}^{\dagger} \otimes U_{2}^{\dagger}$ is in the canonical form. So the MCDM performed on $A$ for an arbitrary two-qubit state is given by

$$\left\{ \frac{1}{2}(1 + U_{1}^{\dagger} \sigma_{1}^{A} U_{1}), \frac{1}{2}(1 - U_{1}^{\dagger} \sigma_{1}^{A} U_{1}) \right\}.$$  

(10)

IV. PERFORMANCE OF THE MCDM

In the following, we will investigate the performance of the MCDM to access the classical correlation measured by the quantum discord.

A. Zero-discord states

The zero-discord states are the states satisfying $\rho = \sum_{k} \Pi_{k}^A \otimes 1_B \rho \Pi_{k}^A \otimes 1_B$, where $\{ \Pi_{k}^A \}$ is just the optimal von Neumann measurement to access the classical correlation, see Ref. [3]. In Appendix A we show that a sufficient and necessary condition of zero-discord is the existence of such a unit vector $n$ satisfying the following equations

$$mn^T a = a,$$

(11)

$$mn^T R = R,$$

(12)

where $a_i = \text{Tr} (\sigma_i^A \rho^A)$ is the polarization vector of the reduced density matrix $\rho^A$. $R$ is a $3 \times 3$ matrix with the elements $R_{ij} = \text{Tr} (\sigma_i^A \otimes \sigma_j^B \rho)$, and $n$ is the column vector characterizing the optimal von Neumann measurement via Eq. [3]. For the states in the canonical form, we have $R = \Lambda + ab^T$, see the definitions of $R$, $\Lambda$, $a$, and $b$. Then the conditions (11) and (12) leads to

$$\Lambda = nn^T \Lambda.$$  

(13)

Considering $\Lambda = \text{diag}\{\Lambda_1, \Lambda_2, \Lambda_3\}$ is a diagonal matrix with $\Lambda_1 \geq \Lambda_2 \geq |\Lambda_3|$, from Eq. (13), the first diagonal element of the matrix $\Lambda$ reads

$$\Lambda_1 = (n_1)^2 \Lambda_1.$$  

(14)

So we obtain $n_1 = \pm 1$, which corresponds to the MCDM.

So we conclude that for the zero-discord states, the MCDM is just the optimal measurement to access the classical correlation.

B. States with maximally mixed marginals

The states with maximally mixed marginals are the ones satisfying $\rho^A = I^A / d_A$ and $\rho^B = I^B / d_B$, where $d_A(B) = \text{dim}(\mathcal{H}^{A(B)})$ is the dimension of the Hilbert-space $\mathcal{H}^{A(B)}$. For two-qubit systems, The canonical forms of states with maximally mixed marginals must be Bell-diagonal states, while an arbitrary Bell-diagonal state need not be in the canonical form. An arbitrary Bell-diagonal state reads

$$\rho = \frac{1}{4} I^A \otimes I^B + \frac{1}{4} \sum_{i=1}^3 c_i \sigma_i^A \otimes \sigma_i^B$$  

(15)

with $c_i = \langle \sigma_i^A \otimes \sigma_i^B \rangle$. Only when $c_1 \geq c_2 \geq |c_3|$, the Bell-diagonal state is in the canonical form. For Bell-diagonal states, Luo got the analytical results of quantum discord [4]. There it was shown that the optimal measurement is given by the unit vector $n = (n_1, n_2, n_3)^T$ which maximizes $\sqrt{\sum_{i=1}^3 c_i^2 n_i^2}$. So the optimal measurements of Bell-diagonal states must be in the universal finite set $\{ \{ (1 \pm \sigma_i^A) / 2 \}_{i=1,2,3} \}$. Here universal means this set of von Neumann measurements is independent on the given states. For the Bell-diagonal states in the canonical form, we have $c_1 \geq c_2 \geq |c_3|$. Then the optimal measurement is explicitly given by $n = (1, 0, 0)^T$, which is consistent with the MCDM [9]. This is because $\Lambda_i = c_i$ due to $\langle \sigma_i^A \rangle = 0$ (maximal mixed marginals), then the maximization of $\sqrt{\sum_{i=1}^3 c_i^2 n_i^2}$ is equivalent to the maximization of $|\Delta_1|^2$, see Eq. (8).

So we conclude that for the states with maximally mixed marginals, the MCDM is just the optimal measurement to access the classical correlation.

C. X-states

In the following, we consider the so-called X-states, named because of the visual appearance of the density
matrix

\[
\rho = \begin{bmatrix}
a & 0 & 0 & w^* \\
b & z^* & 0 & 0 \\
0 & z & c & 0 \\
w & 0 & 0 & d
\end{bmatrix}. \tag{16}
\]

The X-states, including maximally entangled Bell states and Werner states, are a class of typical quantum states in the field of quantum information. An algebraic characterization of X-states is presented in Ref. [51]. The Fano-Bloch representation matrix \(\tau_{ij} = \text{Tr}(\sigma_i^A \otimes \sigma_j^B \rho)\) of X-states is also of X-type

\[
\tau = \begin{bmatrix}
1 & 0 & 0 & b_3 \\
0 & R_{11} & R_{12} & 0 \\
0 & R_{21} & R_{22} & 0 \\
a_3 & 0 & 0 & R_{33}
\end{bmatrix}. \tag{17}
\]

An important property of the class of the X-states is that an X-state after the local unitary operations \(\exp(i\varphi_1^A \varphi_2^B) \otimes \exp(i\varphi_3^A \varphi_2^B)\) is also an X-state. This leads to the following theorem:

**Theorem.** For the X-states, it is impossible to exist a universal finite set of von Neumann measurements among which the optimal measurement must be.

*Proof.* The proof is divided into two steps. First, we assume that for the class of X-state, such a universal finite set exists and is denoted by \(\mathcal{M} := \{\mathcal{M}_i | i \in I\}\), where \(\mathcal{M}_i\) is a von Neumann measurement and \(I\) is a finite set of the indexes. Let \(R_z(\varphi_1, \varphi_2) := R_z(\varphi_1) \otimes R_z(\varphi_2)\) with \(R_z^{A(B)}(\varphi) := \exp(i\varphi A(B)) / 2\). If \(\mathcal{M}_i\) is the optimal measurement for a given state \(\rho\), then \(\mathcal{M}_i(\varphi_1) = R_z(\varphi_1) \mathcal{M}_i R_z(\varphi_1)\) is the optimal measurement for the state \(\tilde{\rho}(\varphi_1, \varphi_2) = R_z(\varphi_1, \varphi_2) \rho R_z(\varphi_1, \varphi_2)\). Because \(\tilde{\rho}(\varphi_1, \varphi_2)\) is also an X-state, we must have \(\mathcal{M}_i(\varphi_1) \in \mathcal{M}\). Remind that \(\mathcal{M}\) is a finite set, the only possibility is that all the \(\mathcal{M}_i\) are invariant under the operation \(R_z(\varphi_1)\) with arbitrary \(\varphi_1\), i.e., the only possibility of \(\mathcal{M}_i\) is \(\{(1 \pm \sigma_3^A) / 2\}\). In the second step, we disprove this only possibility. From Sec. [IV B] we already know that for Bell-diagonal states, there are three possibility of the optimal measurement: \(\{(1 \pm \sigma_3^A) / 2\}\) for \(i = 1, 2, 3\). These three measurements constitute the minimal universal finite set \(\mathcal{M}_{BD}\) of possible optimal measurement for Bell-diagonal states. Because Bell-diagonal states are a subclass of the X-states, \(\mathcal{M}_{BD}\) must be a subset of \(\mathcal{M}\), but actually it is not. This disproves the only possibility derived in the first step. So the above theorem is proved. \(\square\)

The above theorem implies for the entire class of X-states, the optimization procedure involved in the classical correlation must be state-dependent. This result is opposite to that of Ref. [3], where the authors gave a universal finite set of candidates and sought the optimal measurement in this set. In Ref. [54], we show the constraint missed in Ref. [3]. To elucidate this, we also give

\[
\begin{array}{ccc}
\theta & \phi & \text{Percentage} \\
\hline
\pi/2 & 0 & 99.40\% \\
\pi/2 & -\pi/2 & 0.60\%
\end{array}
\]

**TABLE I:** Distribution of the optimal measurements to access the classical correlation, for random density matrices in the canonical form and equivalent to X-states up to local unitary transformations. The total number of the random states is 10000.

an explicit example:

\[
\rho = \begin{bmatrix}
0.0783 & 0 & 0 & 0 \\
0 & 0.1250 & 0.1000 & 0 \\
0 & 0.1000 & 0.1250 & 0 \\
0 & 0 & 0 & 0.6717
\end{bmatrix}. \tag{18}
\]

This state is in the canonical form with \(\Lambda_1 = \Lambda_2 = 0.2\) and \(\Lambda_3 = 0.1479\). The optimal measurements are characterized by two angle \(\theta\) and \(\phi\), via Eq. [4] and

\[
n = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T \tag{19}
\]

with \(\theta \in [0, \pi]\) and \(\phi \in [-\pi/2, -\pi/2]\). It can be directly verified that the state [18] is invariant under the operation \(\exp(i\varphi_1^A \varphi_2^B) \otimes \exp(i\varphi_3^A \varphi_2^B)\), so the optimization is only relevant to \(\theta\), see Ref. [20]. Following the optimization strategy of Ref. [3], the value of \(\theta\) can only be either 0 or \(\pi/2\). However, the optimal measurement of this state is numerically found at \(\theta \approx 0.155\pi\).

In the following, we numerically investigate the probability distribution of the optimal measurement for the class of X-states. We first generate 100,000 random density matrices according to Hilbert-Schmidt measure [52] and then project them into the X-state subspace via \(\rho_X = \sum_{k=1,2} E_k \rho E_k^T\) with \(E_1 = \text{diag}\{1, 0, 0, 1\}\) and \(E_2 = \text{diag}\{0, 1, 1, 0\}\). These random X-states was later transformed into the canonical forms via local unitary transformations. We numerically find optimal measurements to minimize the quantum conditional entropy, utilizing the general expression of the quantum conditional entropy, see Eq. [129] in Appendix [B]. If there are more than one optimal measurement, we chose the one closest to the MCDM, because we concern on how to find an optimal measurement but not all of the optimal measurements. Our numerical results in Table I show the probability that the MCDM would be the optimal measurement is about 99.40%, and the second preference of the optimal measurement is given by \(n = (0, 1, 0)^T\).

In Table I it seems that the value of \(\theta\) for the optimal measurement is always \(\pi/2\), however, a counterexample does exist and is already given in the Eq. [18].

**D. arbitrary two-qubit states**

For arbitrary two-qubit states, the optimization procedure involved in the quantum discord is unreachable up to now. The MCDM solves this optimization for
the states with zero-discord and with maximally mixed marginals. Besides, the MCDM hits the optimal measurements for the most of the X-states. So what about the performance of the MCDM for arbitrary two-qubit states?

We generate 100,000 random density matrices of two qubit according to Hilbert-Schmidt measure \[52\] and transform them into the canonical form. Then we numerically investigate the probability distribution of the optimal measurement characterized by two angle \(\theta\) and \(\phi\) via Eq. (4). In Fig. 1, we show that the MCDM is indeed the preference of the optimal measurements. Meanwhile, the optimal measurements are centralized in the vicinity of the MCDM. This motivates us to consider the MCDM as an alternative of the optimal measurement accessing the classical correlation.

V. MCDM-BASED DISCORD

The centralization of the optimal measurements in the vicinity of the MCDM motivates us to introduce a MCDM-based discord for an arbitrary two-qubit state as follows

\[
\tilde{D}(\rho) := S(\rho_A) - S(\rho) + S(\tilde{\Pi}_A^q)(B|A),
\]

where \(S(\tilde{\Pi}_A^q)(B|A)\) is the quantum conditional entropy \(\sum_k p_k S(\rho_k^B)\) based on the MCDM \(\{\tilde{\Pi}_A^q\}\) given by Eq. (10). Because the MCDM is in the set of von Neumann measurement over which the optimization involved in the quantum discord is taken, \(D(\rho)\) will be not less than the quantum discord \(D(\rho)\). In other words, \(\tilde{D}(\rho)\) is an upper bound of the quantum discord \(D(\rho)\). If \(\tilde{D}(\rho)\) is close enough to \(D(\rho)\), the MCDM-based discord will be a good approximation of the quantum discord. In the following, we investigate how close is the MCDM-based discord to the quantum discord.

First, for simplicity, we consider a family of states \(\rho(q) = (1 - q)|\psi_0\rangle\langle\psi_0| + q|\psi_1\rangle\langle\psi_1|\), which are mixtures of a product state \(|\psi_0\rangle\) and a maximal entangled state \(|\psi_1\rangle\), with the probability \(1 - q\) and \(q\) respectively. Specifically, we choose \(|\psi_0\rangle\) and \(|\psi_1\rangle\) as follows

\[
|\psi_0\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |10\rangle),
\]

\[
|\psi_1\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle).
\]

In Fig. 2 we show that the MCDM-based discord is very close to the quantum discord, which suggest that it can be taken as a good approximation to the quantum discord.

For more convincing arguments, we investigate the MCDM-based discord and the quantum discord for random states. It is shown that for the most of the ran-
dom states, the MCDM-based discord is very close to the quantum discord, see Fig. 3. This demonstrate the efficiency of the MCDM-based discord.

VI. CONCLUSION

In conclusion, we have investigated the probability distribution of the optimal measurement accessing classical correlation and show that the optimal measurements for arbitrary two-qubit state are centralized in the vicinity of the MCDM. We have proved that the MCDM is the very optimal measurement for the states with zero-discord and the ones with maximally mixed marginals. Besides, we have proposed the MCDM-based discord as an upper bound of quantum discord, and demonstrated that the MCDM-based discord could be a good approximation of quantum discord.

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Appendix A: zero-discord state in Fano-Bloch representation

Here, we derive the condition of zero-discord states in the Fano-Bloch representation. An arbitrary two-qubit state can be written in the Fano-Bloch representation as follows [53]:

\[ \rho = \frac{1}{4} \sum_{ij=0}^{3} \tau_{ij} \sigma_i^A \otimes \sigma_j^B \]  

(A1)

where \( \sigma_0^A(B) = 1^A(B) \) is the 2 \( \times \) 2 identity operator, \( \sigma_{1,2,3}^A(B) \) is Pauli matrices. Meanwhile, a von Neumann measurement performed on \( A \) is characterized by a set of von Neumann operators

\[ \Pi_k^A = \frac{1}{2} \sum_{k=0}^{3} \alpha_k \sigma_k^A, \quad \Pi_k^B = \frac{1}{2} \sum_{k=0}^{3} \beta_k \sigma_k^A. \]  

(A2)

The coefficients \( \alpha_k \) and \( \beta_k \) are given by

\[ \alpha_0 = \beta_0 = 1, \quad \alpha_k = -\beta_k = n_k \quad \text{for} \quad k = 1, 2, 3, \]  

(A3)

where \( n_k \) is the \( k \)-th component of the unit vector \( n = (n_1, n_2, n_3)^T \) on Bloch sphere. The zero-discord states are the ones which can be written in the form

\[ \rho = \sum_k p_k \Pi_k^A \otimes \rho_k^B \]  

(A4)

with \( p_k = \text{Tr}(\Pi_k^A \rho) \) and \( \rho_k^B = \text{Tr}_A(\Pi_k^A \rho) / p_k \), see Ref. [3]. With Eq. (A2), \( p_k \) and \( \rho_k^B \) can be obtained via

\[ p_1 \rho_1^B = \frac{1}{4} \sum_{i,j=0}^{3} (\alpha_i \tau_{ij}) \sigma_j^B, \]

\[ p_2 \rho_2^B = \frac{1}{4} \sum_{i,j=0}^{3} (\beta_i \tau_{ij}) \sigma_j^B. \]  

(A5)

Substituting Eqs. (A2) and (A5) into the above form of the zero-discord state (A4), we get

\[ \sum_{ij=0}^{3} \tau_{ij} \sigma_i^A \otimes \sigma_j^B = \frac{1}{2} \sum_{ijk=0}^{3} (\alpha_i \alpha_k + \beta_i \beta_k) \tau_{kj} \sigma_i^A \otimes \sigma_j^B. \]  

(A6)

Because \( \{ \sigma_i^A \otimes \sigma_j^B \} \) is a set of orthogonal basis of operators on \( \mathcal{H}_A \otimes \mathcal{H}_B \), we get

\[ \tau = \frac{1}{2} (\alpha \alpha^T + \beta \beta^T) \tau. \]  

(A7)

where \( \alpha = (\alpha_0, \alpha_1, \alpha_2, \alpha_3)^T \) and \( \beta = (\beta_0, \beta_1, \beta_2, \beta_3)^T \). The matrix \( \tau \) can be further decomposed into

\[ \tau = \begin{bmatrix} 1 & b^T \\ a & R \end{bmatrix}, \]  

(A8)

where \( a, b \) are column vectors and \( R \) are 3 \( \times \) 3 matrix. Combining Eqs. (A3), (A7) and (A8), we obtain the condition of zero-discord states with the Fano-Bloch representation as follows

\[ nn^T a = a, \]  

(A9)

\[ nn^T R = R, \]  

(A10)

where \( n \) is a unit column vector. The existence of such \( n \) satisfying the above equations is a sufficient and necessary condition for the zero-discord.

Appendix B: a general expression of the quantum conditional entropy

In the following, we give a general expression of the quantum conditional entropy in the Fano-Bloch representation. For the states (A1) and the von Neumann measurement (A2), the remaining state of the system \( B \) with measurement result \( k = 1, 2 \) of \( A \) and the corresponding probability are given by Eq. (A3).
To obtain the eigenvalues of $\rho^B_k$, we first get the eigenvalues of $p_k \rho^B_k$. From Eq. (A5), we have

$$\text{eig}(p_k \rho^B_k) = \frac{1}{4} \left( 1 \pm \frac{|b + R^T n|}{1 + a^T n} \right),$$

(B1)

$$\text{eig}(\rho^B_1) = \frac{1}{4} \left( 1 \pm \frac{|b + R^T n|}{1 + a^T n} \right),$$

(B3)

$$\text{eig}(\rho^B_2) = \frac{1}{4} \left( 1 \pm \frac{|b - R^T n|}{1 - a^T n} \right),$$

(B4)

With the decomposition form (A5), we obtain the following results

$$p_1 = \frac{1}{2} (1 + a^T n),$$

(B5)

$$p_2 = \frac{1}{2} (1 - a^T n),$$

(B6)

where $|X|^2 = \text{Tr}(XX^T)$ is the Hilbert-Schmidt norm. By introducing a new set of parameter as follows

$$f(n) = a^T n,$$

(B7)

$$g_{\pm}(n) = |b \pm R^T n|,$$

(B8)

we get the quantum conditional entropy $S_2$ as follows

$$\sum_k p_k S(\rho^B_k) = \frac{1 + f}{2} h \left( \frac{g_+}{1 + f} \right) + \frac{1 - f}{2} h \left( \frac{g_-}{1 - f} \right),$$

(B9)

with $h(x) := -\frac{x + 1}{2} \log_2 \frac{x + 1}{2} - \frac{1 - x}{2} \log_2 \frac{1 - x}{2}$. Then the classical correlation $C$ and the quantum discord $D$ can be obtained via

$$C = S(\rho^B) - \min_{|n|=1} \sum_k p_k S(\rho^B_k),$$

(B10)

$$D = S(\rho^A) - S(\rho) + \min_{|n|=1} \sum_k p_k S(\rho^B_k).$$

(B11)
This conclusion is opposite with the results of Ref. [5]. In Ref. [5], the optimization is taken with respect to the four parameters $m, n, k$ and $l$ with one constraint $k + l = 1$, see Eq. (18) in Ref. [5]. However, only two independent parameters is needed to characterize a von Neumann measurement on two-qubit systems, so there should be one more constraint. The four parameters $m, n, k, l$ are related to three other parameter $z_1, z_2$ and $z_3$ in Ref. [4] through $4m = z_2^2$, $4n = -z_1z_2$, $k - l = z_3$. The three parameters $z_1, z_2, z_3$ satisfy $z_1^2 + z_2^2 + z_3^2 = 1$ [4], which implicitly gives another constraint on the four parameters $m, n, k, l$. This implicit constraint was not taken into consideration in the optimization procedure in Ref. [5]. So the analytical result of quantum discord for X-states has not been obtained up to now.