Necessary and Sufficient Condition for Nonzero Quantum Discord

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Quantum discord characterizes ''nonclassicality'' of correlations in quantum mechanics. It has been proposed as the key resource present in certain quantum communication tasks and quantum computational models without containing much entanglement. We obtain a necessary and sufficient condition for the existence of nonzero quantum discord for any dimensional bipartite states. This condition is easily experimentally implementable. Based on this, we propose a geometrical way of quantifying quantum discord. For two qubits this results in a closed form of expression for discord. We apply our results to the model of deterministic quantum computation with one qubit, showing that quantum discord is unlikely to be the reason behind its speedup.

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Introduction.—Quantum states of a composite system can be divided into entangled and separable ones. Entangled states display ''nonlocal features'' violating Bell's inequalities [1] and are considered a necessary resource for quantum communication and pure quantum computation allowing computational speedup over the best classical algorithm [2]. On the contrary, separable states are generally considered as purely classical, since they do not violate Bell's inequalities and can be prepared by local operations and classical communication. However, it is valid to ask if highly mixed states, and, in particular, separable states, are completely useless from a quantum information perspective. Recent investigations give compelling evidence that this is not the case. A highly mixed state in the deterministic quantum computation with one qubit (DQC1) [3] is believed to perform a task exponentially faster than any classical algorithm (''without containing much entanglement''). Furthermore, it has been shown that even some separable states contain nonclassical correlations [4,5] and can create an advantage for computing and information processing tasks over their classical counterparts [6–11].

The ''nonclassicality'' of bipartite correlations is measured via quantum discord [4]—the discrepancy between quantum versions of two classically equivalent expressions for mutual information. Recently, it has been shown that almost all quantum states have nonvanishing discord [12]. Quantum discord was proposed as a figure of merit for characterizing the nonclassical resources present in the DQC1 [10]. It has been shown that an initial zero-discord system-environment state is a necessary and sufficient condition for completely positive map evolution of the system when the environment is traced out [13,14]. Furthermore, in Ref. [15] it is demonstrated that if the state can be locally broadcasted, it has vanishing discord.

Despite increasing evidence for the relevance of quantum discord in describing nonclassical resources in information processing, there is no direct criterion to verify the presence of discord in a given quantum state. Its evaluation involves optimization procedure, and analytical results are known only in a few cases [16]. In this Letter we derive the necessary and sufficient condition for nonvanishing quantum discord. The criterion is simple and also experimentally friendly, since it can be evaluated directly from a (sub) set of measurements that are standard for quantum state tomography. Based on this, we introduce the geometrical measure of discord and derive an explicit expression for the case of two qubits. Finally, we give arguments that question the appropriateness of quantum discord to describe the nonclassical resource in the DQC1 model.

Quantum discord.—Correlations between two random variables of classical systems A and B are in information theory quantified by the mutual information $I(A{:}B) = H(A) + H(B) - H(A, B)$. If A and B are classical systems, then $H(\cdot)$ stands for the Shannon entropy $H(\mathbf{p}) = -\sum_i p_i \log p_i$, where $\mathbf{p} = (p_1, p_2, \ldots)$ is the probability distribution vector, while $H(.,.)$ is the Shannon entropy of the joint probability distribution p_{ij}. For quantum systems A and B, function $H(\cdot)$ denotes the von Neumann entropy $H(\rho) = -\mathrm{Tr}\rho \log\rho$, where ρ is the density matrix. In the classical case, we can use the Bayes rule and find an equivalent expression for the mutual information $I(A{:}B) = H(A) - H(A|B)$, where $H(A|B)$ is the Shannon entropy of A conditioned on the measurement outcome on B. For quantum systems, this quantity is different from the first expression for the mutual information and the difference defines the quantum discord.

Consider a quantum composite system defined by the Hilbert space $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. Let dimensions of the local Hilbert spaces be $\dim \mathcal{H}_{\mathcal{A}} = d_A$ and $\dim \mathcal{H}_{\mathcal{B}} = d_B$, while $d = \dim \mathcal{H}_{\mathcal{AB}} = d_A d_B$. Given a state ρ (density matrix) of a composite system, the total amount of correlations is quantified by quantum mutual information [17]:

$$I(\rho) = H(\rho_A) + H(\rho_B) - H(\rho), \qquad (1)$$

where $H(\rho)$ is the von Neumann entropy and $\rho_{A,B} = \mathrm{Tr}_{B,A}(\rho)$ are reduced density matrices. A generalization of the classical conditional entropy is $H(\rho_{B|A})$, where $\rho_{B|A}$ is the state of B given a measurement on A. By optimizing over all possible measurements in A, we define an alternative version of the mutual information

$$Q_A(\rho) = H(\rho_B) - \min_{\{E_k\}} \sum_k p_k H(\rho_{B|k}), \qquad (2)$$

where $\rho_{B|k} = \mathrm{Tr}_A(E_k \otimes \mathbb{1}_B \rho)/\mathrm{Tr}(E_k \otimes \mathbb{1}_B \rho)$ is the state of B conditioned on outcome k in A, and $\{E_k\}$ represents the set of positive operator valued measure elements. The discrepancy between the two measures of information defines the quantum discord [4,5]:

$$D_A(\rho) = I(\rho) - Q_A(\rho). \qquad (3)$$

The discord is always non-negative [4] and reaches zero for the classically correlated states [5]. Note that discord is not a symmetric quantity $D_A(\rho) \neq D_B(\rho)$ and D_A refers to the ''left'' discord, while D_B refers to the ''right'' discord. The state ρ for which $D_A(\rho) = D_B(\rho) = 0$ is *completely* classically correlated in the sense of [18,19]. From now on, when we refer to the discord we mean the ''left'' discord D_A.

To give an example of a state with nonvanishing discord, consider the two-qubit separable state in which four nonorthogonal states of one qubit are correlated with four nonorthogonal states of the second qubit:

$$\tfrac{1}{4}(|0\rangle\langle 0| \otimes |+\rangle\langle +| + |1\rangle\langle 1| \otimes |-\rangle\langle -| + |+\rangle\langle +| \otimes |1\rangle\langle 1| + |-\rangle\langle -| \otimes |0\rangle\langle 0|). \qquad (4)$$

Unlike the state above, one can show that the state ρ is of zero discord if and only if there exists a von Neumann measurement $\{\Pi_k = |\psi_k\rangle\langle\psi_k|\}$ such that [20]

$$\sum_k (\Pi_k \otimes \mathbb{1}_B)\rho(\Pi_k \otimes \mathbb{1}_B) = \rho. \qquad (5)$$

In other words, the zero-discord state is of the form $\rho = \sum_k p_k |\psi_k\rangle\langle\psi_k| \otimes \rho_k$, where $\{|\psi_k\rangle\}$ is some orthonormal basis set, ρ_k are the quantum states in B, and p_k are non-negative numbers such that $\sum_k p_k = 1$.

Easily implementable necessary and sufficient condition.—Let us choose basis sets in local Hilbert-Schmidt spaces of Hermitian operators, $\{A_n\}$ and $\{B_m\}$ where $n = 1, \ldots, d_A^2$ and $m = 1, \ldots, d_B^2$. We decompose the state ρ of the composite system into $\rho = \sum_{nm} r_{nm} A_n \otimes B_m$. The coefficients r_{nm} define $d_A^2 \times d_B^2$ real matrix R, which we call the correlation matrix. We can find its singular value decomposition (SVD), $URW^T = \mathrm{diag}[c_1, c_2, \ldots]$ where U and W are $d_A^2 \times d_A^2$ and $d_B^2 \times d_B^2$ orthogonal matrices, respectively, while $\mathrm{diag}[c_1, c_2, \ldots]$ is $d_A^2 \times d_B^2$ diagonal matrix. SVD defines the new basis in local spaces $S_n = \sum_{n'} U_{nn'} A_{n'}$ and $F_m = \sum_{m'} W_{mm'} B_{m'}$. The state ρ in the new basis is of the form $\rho = \sum_{n=1}^{L} c_n S_n \otimes F_n$, where $L = \mathrm{rank}\, R$ is the rank of correlation matrix R (the number of nonzero eigenvalues c_n).

The necessary and sufficient condition (5) becomes $\sum_{n=1}^{L} c_n (\sum_k \Pi_k S_n \Pi_k) \otimes F_n = \sum_{n=1}^{L} c_n S_n \otimes F_n$ and it is equivalent to the set of conditions:

$$\sum_k \Pi_k S_n \Pi_k = S_n, \qquad n = 1, \ldots, L, \qquad (6)$$

or equivalently $[S_n, \Pi_k] = 0$ for all k, n. This means that the set of operators $\{S_n\}$ has a common eigenbasis defined by the set of projectors $\{\Pi_k\}$. Therefore, the set $\{\Pi_k\}$ exists if and only if

$$[S_n, S_m] = 0, \qquad n, m = 1, \ldots, L. \qquad (7)$$

In order to show zero discord we have to check at most $L(L-1)/2$ commutators, where $L = \mathrm{rank}\, R \leq \min\{d_A^2, d_B^2\}$. Now, recall that the state of zero discord is of the form $\rho = \sum_{k=1}^{d_A} p_k \Pi_k \otimes \rho_k$; therefore, it is a sum of at most d_A product operators. This bounds the rank of the correlation tensor to $L \leq d_A$. Thus, the rank of the correlation tensor is the simple discord witness: If $L > d_A$, the state has a nonzero discord.

A correlation matrix can be obtained directly by simple measurements usually involved in quantum state tomography. However, the detection of nonzero discord does not necessarily require measurement of all $(d_A d_B)^2$ elements of the correlation matrix (full state tomography). It is sufficient that the experimentalist measures that many elements of the correlation matrix until he finds $d_A + 1$ linearly independent rows (or columns) of the correlation matrix.

Geometric measure of discord.—Evaluation of quantum discord given by Eq. (3) in general requires considerable numerical minimization. Different measures of quantum discord [21] and their extensions to multipartite systems [19] have been proposed. However, analytical expression are known only for certain classes of states [16]. Here we propose the following geometric measure,

$$D_A^{(2)}(\rho) = \min_{\chi \in \Omega_0} \|\rho - \chi\|^2, \qquad (8)$$

where Ω_0 denotes the set of zero-discord states and $\|X - Y\|^2 = \mathrm{Tr}(X - Y)^2$ is the square norm in the Hilbert-Schmidt space. We will show how to evaluate this quantity for an arbitrary two-qubit state.

Two-qubit case.—Consider the case $\mathcal{H}_A = \mathcal{H}_B = \mathbb{C}^2$. We write a state ρ in Bloch representation:

$$\rho = \frac{1}{4}\left(\mathbb{1} \otimes \mathbb{1} + \sum_{i=1}^{3} x_i \sigma_i \otimes \mathbb{1} + \sum_{i=1}^{3} y_i \mathbb{1} \otimes \sigma_i + \sum_{i,j=1}^{3} T_{ij} \sigma_i \otimes \sigma_j\right), \qquad (9)$$

where $x_i = \mathrm{Tr}\rho(\sigma_i \otimes \mathbb{1})$, $y_i = \mathrm{Tr}\rho(\mathbb{1} \otimes \sigma_i)$ are components of the local Bloch vectors, $T_{ij} = \mathrm{Tr}\rho(\sigma_i \otimes \sigma_j)$ are components of the correlation tensor, and σ_i, $i \in \{1, 2, 3\}$, are the three Pauli matrices. To each state ρ we associate the triple $\{\vec{x}, \vec{y}, T\}$. Now, we characterize the set Ω_0. A zero-discord state is of the form $\chi = p_1|\psi_1\rangle\langle\psi_1| \otimes \rho_1 + p_2|\psi_2\rangle\langle\psi_2| \otimes \rho_2$, where $\{|\psi_1\rangle, |\psi_2\rangle\}$ is a single-qubit orthonormal basis, $\rho_{1,2}$ are 2×2 density matrices, and $p_{1,2}$ are non-negative numbers such that $p_1 + p_2 = 1$. We define $t = p_1 - p_2$ and three vectors

$$\vec{e} = \langle\psi_1|\vec{\sigma}|\psi_1\rangle, \tag{10}$$

$$\vec{s}_{\pm} = \mathrm{Tr}(p_1\rho_1 \pm p_2\rho_2)\vec{\sigma}. \tag{11}$$

It can easily be shown that $t\vec{e}$ and $\vec{s}_+$ represent the local Bloch vectors of the first and second qubit, respectively, while the vector $\vec{s}_-$ is directly related to the correlation tensor which is of the product form $T = \vec{e}\vec{s}_-^T$. Therefore, a state of zero discord χ has Bloch representation $\vec{\chi} = \{t\vec{e}, \vec{s}_+, \vec{e}\vec{s}_-^T\}$, where $\|\vec{e}\| = 1$, $\|\vec{s}_{\pm}\| \leq 1$, and $t \in [-1, 1]$. The distance between states ρ and χ is given by

$$\begin{aligned}\|\rho - \chi\|^2 &= \|\rho\|^2 - 2\,\mathrm{Tr}\rho\chi + \|\chi\|^2 \\ &= \tfrac{1}{4}(1 + \|\vec{x}\|^2 + \|\vec{y}\|^2 + \|T\|^2) \\ &\quad - \tfrac{1}{2}(1 + t\vec{x}\,\vec{e} + \vec{y}\vec{s}_+ + \vec{e}T\vec{s}_-) \\ &\quad + \tfrac{1}{4}(1 + t^2 + \|\vec{s}_+\|^2 + \|\vec{s}_-\|^2),\end{aligned} \tag{12}$$

where $\|T\|^2 = TrT^TT$. First, we optimize the distance over parameters $\vec{s}_{\pm}$ and t. The function of Eq. (12) is convex and quadratic in its variables $t, \vec{s}_{\pm}$. It is straightforward to see that its Hessian is a positive and nonsingular matrix. Therefore, the function has a unique global minimum. The minimum occurs when the derivative is zero:

$$\frac{\|\rho - \chi\|^2}{\partial t} = \frac{1}{2}(-\vec{x}\,\vec{e} + t) = 0, \tag{13}$$

$$\frac{\|\rho - \chi\|^2}{\partial \vec{s}_+} = \frac{1}{2}(-\vec{y} + \vec{s}_+) = 0, \tag{14}$$

$$\frac{\|\rho - \chi\|^2}{\partial \vec{s}_-} = \frac{1}{2}(-T^T\vec{e} + \vec{s}_-) = 0, \tag{15}$$

which gives the solution $t = \vec{x}\,\vec{e}$, $\vec{s}_- = \vec{y}$, and $\vec{s}_+ = T^T\vec{e}$. Since the solution lies within the range of parameters, $|\vec{x}\,\vec{e}|, \|\vec{y}\|, \|T^T\vec{e}\| \leq 1$ it represents the global minimum. After substituting the solution we obtain $\|\rho - \chi\|^2 = \frac{1}{4}[\|\vec{x}\|^2 + \|T\|^2 - \vec{e}(\vec{x}\vec{x}^T + TT^T)\vec{e}]$, which attains the minimum when $\vec{e}$ is an eigenvector of matrix $K = \vec{x}\vec{x}^T + TT^T$ for the largest eigenvalue. Therefore, we have

$$D_A^{(2)}(\rho) = \tfrac{1}{4}(\|\vec{x}\|^2 + \|T\|^2 - k_{\max}), \tag{16}$$

where $k_{\max}$ is the largest eigenvalue of matrix $K = \vec{x}\vec{x}^T + TT^T$. Next, we apply our criterion to a class of states.

States with maximally mixed marginals.—We consider an example of two qubit states with maximally mixed marginals. Such a state is locally equivalent (under some local unitary transformation $U_1 \otimes U_2$) to a state $\rho(\vec{t}) = (\mathbb{1} \otimes \mathbb{1} + \sum_{i=1}^{3} t_i\sigma_i \otimes \sigma_i)/4$, where $\vec{t} = (t_1, t_2, t_3)$. The state $\rho(\vec{t})$ is physical if $\vec{t}$ belongs to the tetrahedron (Fig. 1) defined by the set of vertices $(-1, -1, -1)$, $(-1, 1, 1)$, $(1, -1, 1)$, and $(1, 1, -1)$, while is separable if $\vec{t}$ belongs to the octahedron defined by the set of vertices $(\pm1, 0, 0)$, $(0, \pm1, 0)$, and $(0, 0, \pm1)$ [22]. Simple calculation shows that $D_A^{(2)}(\vec{t}) = \frac{1}{4}(t_1^2 + t_2^2 + t_3^2 - \max\{t_1^2, t_2^2, t_3^2\})$. The zero-discord states have at most one nonzero component of vector $\vec{t}$ [Fig. 1, solid gray (red) lines]. The function $D_A^{(2)}(\vec{t})$ reaches its maximal value of $D_A^{(2)} = 1/2$ at the vertices of tetrahedron which represent the four Bell states. Within the set of separable states (octahedron) its maximal value of $D_A^{(2)} = 1/6$ is attained at the centers of octahedron facets $(\pm1, \pm1, \pm1)/3$. They represent the states

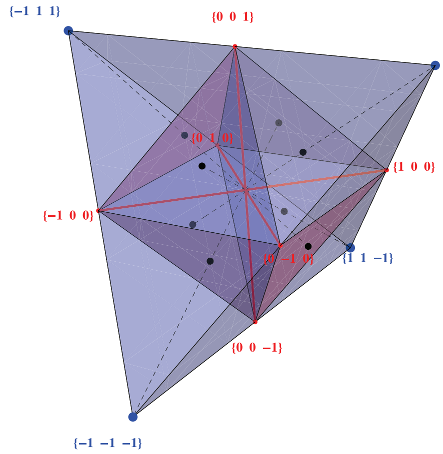

FIG. 1 (color online). The set of two-qubit states with maximally mixed marginals (i.e., the reduced states of individual qubits are completely mixed). Physical states belong to the tetrahedron, among which separable ones are confined to the octahedron. The zero-discord states are labeled by the solid gray (red) lines (almost all states have nonzero discord [12]). The states with maximal value of discord correspond to the vertices of the tetrahedron (the four Bell states). Among the set of separable states, those which maximize discord are the centers of octahedron facets $(\pm1, \pm1, \pm1)/3$ (black dots).

$$\rho_{i_1i_2i_3} = \frac{1}{4}\left(\mathbb{1} \otimes \mathbb{1} + \frac{1}{3}\sum_{k=1}^{3}(-1)^{i_k}\sigma_k \otimes \sigma_k\right), \tag{17}$$

where $i_k = \pm1$ and can intuitively be understood as equal mixture of "maximally nonorthogonal" states. The states are symmetric under exchange of subsystems; thus, they have the same value of left and right discord $D_A = D_B$.

DQC1 model.—In [3], Knill and Laflamme introduced the model of mixed-state quantum computing which preforms the task of evaluating the normalized trace of a unitary matrix efficiently. The corresponding quantum circuit is shown in Fig. 2. The input state is a highly mixed separable state and consists of a control qubit in the state $\frac{1}{2}(\mathbb{1} + \alpha\sigma_3)$, where α describes the purity, and a collection of n qubits in the maximally mixed state $\frac{1}{2^n}\mathbb{1}_n$, where $\mathbb{1}_n$ is the n-qubit identity. The DQC1 circuit consists of the Hadamard gate applied to the control qubit and a control n-qubit unitary gate U_n. The output state is

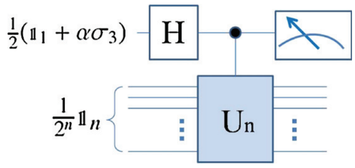

FIG. 2 (color online). The quantum circuit for estimating the normalized trace of the unitary matrix U_n using the model of deterministic computing with one quantum bit (DQC1). H stands for the Hadamard gate. The control (top) qubit is measured in the σ_1 and σ_2 basis, and the expectation values give the real and imaginary parts of normalized trace $\tau = \mathrm{Tr}U_n/2^n$ with the overhead scaling as $\frac{1}{\alpha^2}$ [10].

$$\rho = \frac{1}{2^{n+1}}(\mathbb{1}_1 \otimes \mathbb{1}_n + \alpha|1\rangle\langle 0| \otimes U_n + \alpha|0\rangle\langle 1| \otimes U_n^\dagger). \quad (18)$$

We consider only the cases $\alpha \neq 0$; otherwise, the state at the output is completely mixed and therefore cannot accomplish the task. After measuring the control qubit at the output in the eigenbasis of σ_1 and σ_2, we retrieve the normalized trace of the unitary matrix $\tau = \mathrm{Tr}U_n/2^n$ with the polynomial overhead scaling $1/\alpha^2$ [10].

The control qubit is completely separable from the rest of the qubits. The output state has vanishingly small entanglement across any bipartite split that groups the control qubit with some of the mixed qubits [3]. However, there is strong evidence that a DQC1 task cannot be preformed efficiently using classical computation [9]. The question is, what brings a "speedup" in the considered task? The quantum discord was proposed as a figure of merit for characterizing the resources present in the DQC1 model [10]. It has been shown that for almost every unitary matrix U_n (random unitary) the discord in the output state (18) is nonvanishing. Here we derive an explicit condition for characterizing the correlations in the output state and show that the discord is unlikely to be the source of speedup. We rewrite it into the following form:

$$\rho = \frac{1}{2^{n+1}}\left(\mathbb{1}_1 \otimes \mathbb{1}_n + \alpha\sigma_1 \otimes \frac{U_n + U_n^\dagger}{2} + \alpha\sigma_2 \otimes \frac{U_n - U_n^\dagger}{2i}\right). \quad (19)$$

Now, we apply the condition (7). The operators σ_1 and σ_2 do not commute; therefore, the state ρ is of the zero discord if and only if the operators $\frac{U_n+U_n^\dagger}{2}$ and $\frac{U_n-U_n^\dagger}{2i}$ are linearly dependent, or equivalently, $U_n^\dagger = kU_n$. This is possible if and only if $U_n = e^{i\phi}A$, where $A^2 = A$ is a binary observable. For such a unitary all the correlations at the output of the DQC1 circuit are classical. However, it is very unlikely that the normalized trace of $e^{i\phi}A$ can be evaluated efficiently on a classical computer, since all of its eigenvectors can be arbitrarily complex (random states).

We emphasize that our measure of discord is not monotonic under local operations. This, however, is not a shortcoming, as discord, unlike entanglement and mutual information, can in fact increase as well as decrease under local operations (even without the presence of classical correlations). A simple example of the local increase is to start from a zero-discord state $|00\rangle\langle 00| + |11\rangle\langle 11|$ and transform, say, the first qubit, so that $|0\rangle \rightarrow |\psi_0\rangle$ and $|1\rangle \rightarrow |\psi_1\rangle$, such that $|\psi_0\rangle$ and $|\psi_1\rangle$ are not orthogonal. The resulting state, $|0\Psi_0\rangle\langle 0\Psi_0| + |1\psi_1\rangle\langle 1\psi_1|$, clearly has a nonvanishing discord. Finally, we point out that our method can be extended to any number of subsystems, though evaluating the measure of discord becomes progressively more difficult with increasing number of subsystems and their dimensionality.

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Note added in proof.—A related work was done by Datta [23].

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