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Reveal quantum correlation in complementary bases

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An essential feature of genuine quantum correlation is the simultaneous existence of correlation in complementary bases. We reveal this feature of quantum correlation by defining measures based on invariance under a basis change. For a bipartite quantum state, the classical correlation is the maximal correlation present in a certain optimum basis, while the quantum correlation is characterized as a series of residual correlations in the mutually unbiased bases. Compared with other approaches to quantify quantum correlation, our approach gives information-theoretical measures that directly reflect the essential feature of quantum correlation.

uantum physics differs significantly from classical physics in many aspects. A complete classical description of an object contains information concerning only compatible properties, while a complete quantum description of an object also contains complementary information concerning incompatible properties (see Fig. 1). This difference is also present in correlations. A classical correlation in a bipartite system involves the correlation of only a certain property, while a quantum correlation in a bipartite system also involves complementary correlations of incompatible properties. The simultaneous existence of complementary correlations together with the freedom to select which one to extract is the most important feature of quantum correlation (see Fig. 2). Schrödinger introduced the word "entanglement" to describe this peculiar feature, which was termed "spooky action at a distance" by Einstein¹⁻⁴.

More recently, entangled states were defined as states that cannot be written as convex sums of product states. This precise definition is very helpful in terms of both mathematical and physical convenience, and it motivates the useful definition of the entanglement of formation. However, we now know that entanglement of formation is just one particular aspect of quantum correlation. Many measures of quantum correlation have been proposed from different perspectives, and they can be divided into two categories: entanglement measures^{5–9}, and measures of nonclassical correlation beyond entanglement^{10–24}.

The essential feature of quantum correlation, i.e., the simultaneous existence of complementary correlations in different bases, is also revealed by the Bell's inequalities^{25,26}. Bell's inequalities quantify quantum correlation via expectation values of local complementary observables. Instead, we shall seek a way to directly reveal the essential feature of quantum correlation from an information-theoretical perspective. Indeed, there are several previous entropic measures of quantum correlation (such as quantum discord *D*, measurement-induced disturbance, symmetric discord, etc), which are proposed from an information-theoretical perspective. But these measures are based on the difference between quantum mutual information²⁷ (which is assumed as the total correlation) and a certain measure of classical correlation. Here, we take a different approach and reveal the essential feature of quantum correlation directly. The genuine quantum correlation does not vanish under a change of basis, and can be characterized as the residual correlations remaining in the complementary bases.

Results

The idea. We begin with a comparison between the correlations in two different states:

$$\rho_{c} = \frac{1}{2} (|00\rangle \langle 00| + |11\rangle \langle 11|), \qquad (1)$$



Figure 1 (a) A complete classical description of a classical object (a giraffe) is a simple collection of information about compatible properties, such as color, height, weight, position and velocity (the photo was taken by S.W. in Hefei animal zoo). (b) A complete quantum description (a quantum state $|\psi\rangle$) of a quantum system (e.g. a spin-1/2 particle) contains information about incompatible properties ($\sigma_x \sigma_y, \sigma_z$) in an intrinsic way: information about incompatible properties exists simultaneously even though only a single property can be measured at a time; and we can freely select which property to measure.

$$|EPR\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \tag{2}$$

The first state has only classical correlation, which can be revealed when Alice and Bob each measure the observable σ_{z^3} i.e., project their qubits onto the basis { $|0\rangle$, $|1\rangle$ }. If they measure a complementary observable, σ_x or σ_y , no correlation between their measurement results exists. The second state is the Einstein-Podolsky-Rosen (EPR) state (or the singlet state), which has both classical and quantum correlations. The classical correlation in the EPR state can be revealed when Alice and Bob each measure the same observable, e.g. σ_z . Moreover, this kind of correlation also exists simultaneously in complementary bases (actually, in all bases). The simultaneous existence of correlation in complementary bases is an essential feature of the genuine quantum correlation. This feature is illustrated in Fig. 2 and treated in a rigorous manner in the rest of this article.

Classical and genuine quantum correlations. For any bipartite quantum state ρ_{AB} , there are many measures of classical correlation²⁸. Here, we use the one proposed by Henderson and Vedral²⁹, which is also used in the definition of quantum discord¹⁰. Alice selects a basis $\{|a_i\rangle_A | i=1, \cdots, d_A\}$ of her system in a d_A -dimensional Hilbert space and performs a measurement projecting her system onto the basis states. With probability $p_i = tr_{AB}((|a_i\rangle_A))$ $\langle a_i | \otimes I_B \rangle \rho_{AB}$, Alice will obtain the *i*-th basis state $|a_i\rangle$, and Bob's system will be left in the corre sponding state $\rho_i^B = A \langle a_i | \rho_{AB} |$ $a_i\rangle_A/p_i$. The Holevo quantity of the ensemble $\{p_i, \rho_i^B\}$ that is prepared for Bob by Alice via her local measurement is given by $\chi\{\rho_{AB}|\{|a_i\rangle_A\}\} = \chi\{p_i;\rho_i^B\} \equiv S\left(\sum_i p_i\rho_i^B\right) - \sum_i p_i S(\rho_i^B), \text{ which}$ denotes the upper bound of Bob's accessible information about Alice's measurement result when Alice projects her system onto the basis $\{|a_i\rangle_A\}$. The classical correlation in the state ρ_{AB} is defined as the maximal Holevo quantity over all local projective measurements on Alice's system:

$$C_1(\rho_{AB}) \equiv \max_{\{|a_i\rangle_A\}} \chi\{\rho_{AB} |\{|a_i\rangle_A\}\}.$$
(3)

A basis $\{|a_i\rangle_A\}$ that achieves the maximum $C_1(\rho_{AB})$ is called a C_1 -basis of ρ_{AB} , and is denoted as $\{|\mathcal{A}_i^1\rangle_A | i=1, \cdots, d_A\}$. There could exist many C_1 -bases for a state ρ_{AB} .

We consider another basis $\left\{ \left| a_j^2 \right\rangle_A | j = 1, \cdots, d_A \right\}$, which is mutually unbiased to the C_1 -basis $\left\{ \left| \mathcal{A}_i^1 \right\rangle_A | i = 1, \cdots, d_A \right\}$ in the sense that $\left| \left\langle \mathcal{A}_i^1 \right| a_j^2 \right\rangle \right| = \frac{1}{\sqrt{d_A}}$, i.e., if the system is in a state of one basis, a projective measurement onto the mutually unbiased basis (MUB)



Figure 2 | (a) Classical correlation in a bipartite state reaches the maximum in a certain basis and vanishes in any complementary basis.
(b) However, quantum correlation in a bipartite state contains correlations in complementary bases simultaneously; and one can freely select with which basis to read out the correlation.

will yield each basis state with the same probability. The most essential feature of quantum correlation is that when Alice performs a measurement in another basis $\left\{ \left| a_{j}^{2} \right\rangle_{A} \left| j = 1, \cdots, d_{A} \right. \right\}$ that is mutually unbiased to the C_{1} basis, Bob's accessible information about Alice's results, characterized by the Holevo quantity, does not vanish. This residual correlation represents genuine quantum correlation and can be used as a measure of the quantum correlation. Formally, a measure of quantum correlation $Q_{2}(\rho_{AB})$ in the state ρ_{AB} is defined as the Holevo quantity of Bob's accessible information about Alice's results, maximized over Alice's projective measurements in the bases that are mutually unbiased to a C_{1} -basis $\left\{ \left| \mathcal{A}_{i}^{1} \right\rangle_{A} \right| i = 1, \cdots, d_{A} \right\}$, and further maximized over all possible $\left\{ \left| \mathcal{A}_{i}^{1} \right\rangle_{A} \right\}$ (if not unique), i.e.,

$$Q_2(\rho_{AB}) \equiv \max_{\left\{ \left| \mathcal{A}_i^1 \right\rangle_A \right\}} \max_{\left\{ \left| a_j^2 \right\rangle_A \right\}} \chi \left\{ \rho_{AB} \left| \left\{ \left| a_j^2 \right\rangle_A \right\} \right\} \right\}.$$
(4)

where $\left\{ \left| a_{j}^{2} \right\rangle_{A} | j = 1, \cdots, d_{A} \right\}$ is any basis mutually unbiased to the basis $\left\{ \left| A_{i}^{2} \right\rangle_{A} | i = 1, \cdots, d_{A} \right\}$. A basis $\left\{ \left| a_{j}^{2} \right\rangle_{A} \right\}$ that achieves the maximum quantum correlation Q_{2} in (4) is called a Q_{2} -basis, and is denoted as $\left\{ \left| A_{j}^{2} \right\rangle_{A} | j = 1, \cdots, d_{A} \right\}$. If there is only one C_{1} -basis, the second maximization over the C_{1} -bases $\left\{ \left| A_{i}^{1} \right\rangle_{A} \right\}$ in (4) is not necessary. If there is more than one C_{1} -basis, and not all of them achieve the maximum in (4), then we redefine the C_{1} -bases as those that also achieve the maximum in (3) but do not achieve the maximum in (4) will not be considered as $\left\{ \left| A_{i}^{1} \right\rangle_{A} \right\}$ any more. After this redefinition, if $\left\{ \left| A_{i}^{1} \right\rangle_{A} \right\}$ is still not unique, then $\left\{ \left| A_{j}^{2} \right\rangle_{A} \right\}$ depends on the choice of $\left\{ \left| A_{i}^{1} \right\rangle_{A} \right\}$. It is also obvious that $\left\{ \left| A_{j}^{2} \right\rangle_{A} \right\}$ is mutually unbiased to $\left\{ \left| A_{i}^{1} \right\rangle_{A} \right\}$.

Similar to the case of characterizing entanglement, a single quantity is not sufficient to describe the full property of quantum correlation because there could be many types of quantum correlation. Following the same line of reasoning, we can define the residual correlation in a third MUB as

$$Q_{3}(\rho_{AB}) \equiv \max_{\left\{\left|\mathcal{A}_{i}^{1}\right\rangle_{A}\right\}} \max_{\left\{\left|\mathcal{A}_{j}^{2}\right\rangle_{A}\right\}} \max_{\left\{\left|a_{k}^{3}\right\rangle_{A}\right\}} \chi\left\{\rho_{AB}\left|\left\{\left|a_{k}^{3}\right\rangle_{A}\right\}\right\}\right\}, \quad (5)$$

where $\left\{ |a_k^3\rangle_A | k = 1, \cdots, d_A \right\}$ is any basis mutually unbiased to both $\left\{ |\mathcal{A}_i^1\rangle_A \right\}$ and $\left\{ |\mathcal{A}_j^2\rangle_A \right\}$. An optimum basis $\left\{ |a_k^3\rangle_A \right\}$ to achieve the maximum in (5) is called a Q₃-basis, and is denoted as $\left\{ |\mathcal{A}_k^3\rangle_A | k = 1, \cdots, d_A$. Similarly, we redefine the Q₂-bases $\left\{ |\mathcal{A}_j^2\rangle_A \right\}$ as those that are optimum in both (4) and (5), and further redefine the C₁-bases $\left\{ |\mathcal{A}_i^1\rangle_A \right\}$ as those that are optimum in (3), (4) and (5).

Suppose in this manner that we can define M quantities for the measures of correlation, which are conveniently written as a single correlation vector $\vec{C} \equiv (C_1, Q_2, Q_3, \dots, Q_M)$ for the state ρ_{AB} . The number M cannot be greater than the number of MUBs that exist in the d_A -dimensional Hilbert space. The first quantity C_1 denotes the maximal classical correlation present in the state ρ_{AB} , which can be revealed when Alice performs a measurement of her system in a C_1 -basis $\left\{ |\mathcal{A}_i^1\rangle_A | i=1, \dots, d_A \right\}$. As classical correlation will vanish when measured in a mutually unbiased basis, all of the other quantities describe genuine quantum types of correlation. The second quantity Q_2 denotes the maximal genuine quantum correlation, and $\left\{ |\mathcal{A}_j^2\rangle_A | j=1, \dots, d_A \right\}$ denotes an optimum basis to reveal this correlation. The third quantity Q_3 denotes another type of genuine quantum correlation, and $\left\{ |\mathcal{A}_k^3\rangle_A | j=1, \dots, d_A \right\}$ denotes a basis to reveal the second type of quantum correlation.

The splitting of the correlation vector as a single classical component (C_1) and several quantum components (Q_2, \dots, Q_M) is not artificial, in fact, this splitting captures the essential difference between classical correlation and quantum correlation. The quantity C_1 represents the maximal amount of correlation available in a single basis $\left(\left\{\left|\mathcal{A}_{i}^{1}\right\rangle_{A}\right\}\right)$. The quantity Q_{2} represents the maximal amount of correlation that is available not only in the first basis $\left\{ \left| \mathcal{A}_{i}^{1} \right\rangle_{A} \right\}$ but also in a second complementary basis $\left\{ \left| \mathcal{A}_{j}^{2} \right\rangle_{A} \right\}$ (we know $C_1 \ge Q_2 \ge Q_3 \ge \cdots$ from the definition of these quantities). And Q_3 represents the maximal amount of correlation available not only in $\left\{ \left| \mathcal{A}_{i}^{1} \right\rangle_{A} \right\}$ and $\left\{ \left| \mathcal{A}_{j}^{2} \right\rangle_{A} \right\}$, but also in a third MUB $\left\{ \left| \mathcal{A}_{k}^{3} \right\rangle_{A} \right\}$. The amount Q₃ of correlation exists in 3 MUBs while the amount Q₂ of correlation may only exist in 2 MUBs. Thus, Q3 represents the amount of correlation with a higher level of quantumness than that of Q₂, and may have more practical advantages when 3 MUBs are necessarily used (e.g. entanglement-based QKD via 6-state protocol).

It should be pointed out that the maximum number of MUBs that exist in a d_A -dimensional Hilbert space is not known for the general case. When d_A is a power of a prime number, a full set of $d_A + 1$ MUBs exists; for other cases, there may not exist $d_A + 1$ MUBs. For example, when $d_A = 6$, only 3 MUBs have been found yet, while 3 is much less than $d_A + 1 = 7$. Many interesting works can be found on the existence of MUBs in the literature³⁰⁻³⁴. Since there exist at least 3 MUBs for any integer $d_A \ge 2$, the quantities C_1 , Q_2 , and Q_3 are welldefined for any $d_A \ge 2$. In many cases, we are interested in combined systems of qubits with d_A being a power of 2, thus, $d_A + 1$ MUBs exist and quantities $C_1, Q_2, \dots, Q_{d_A+1}$ are all well-defined. For an arbitrary d_A -dimensional Hilbert space, we don't make assumptions about the maximal number of MUBs that exist, we only assume that M MUBs are available, where M is less or equal to the maximal number of MUBs that exist. In many cases, we only discuss the first 3 elements $(C_1, Q_2, \text{ and } Q_3)$ of the correlation vector for simplicity.

Examples. Now, we shall calculate the correlation vector for several families of bipartite states, and see how these measures in terms of MUBs are well justified as measures of classical and genuine quantum correlations.

For a bipartite pure state written in the Schmidt basis, $|\psi\rangle_{AB} = \sum_i \sqrt{\lambda_i} |a_i\rangle |b_i\rangle$, the maximal classical correlation can be revealed when Alice performs her measurement onto her Schmidt basis { $|a_i\rangle$ }; thus, one immediately has $C_1 = S(\rho_B) = \sum_i -\lambda_i \log_2 \lambda_i$. If Alice chooses another basis { $|a'_i\rangle$ }, whenever she obtains a particular measurement result, Bob will be left with a pure state. Therefore, one can easily obtain the maximal true quantum correlation $Q_2 = S(\rho_B) = C_1$; any other basis will yield the same amount of quantum correlation. Therefore, the correlation vector for a bipartite pure state $|\psi\rangle_{AB}$ is given as $\vec{C} = (S(\rho_B), S(\rho_B), \dots, S(\rho_B))$. The correlation vector exhibits a unique feature of the correlations in a pure state: the classical correlation is equal to the quantum correlation revealed in any basis, and both values are equal to the von Neumann entropy of the reduced density matrix on either side, which is the usual measure of entanglement in a pure state.

A classical-quantum (CQ) state is a bipartite state that can be written as

$$\rho^{cq} = \sum_{i} q_i |i\rangle \langle i| \otimes \sigma_i, \tag{6}$$

where $\{q_i\}$ is a probability distribution, $\{|i\rangle|i=0,1,\cdots,d_A-1\}$ is a basis of system A in a d_A -dimensional Hilbert space, and $\{\sigma_i\}$ is a set of density matrices of system B. The maximal classical correlation is revealed when Alice performs her measurement in the basis $\{|i\rangle\}^{12}$; thus, the maximal classical correlation in the CQ state ρ^{cq} is given by $C_1 = \chi\{q_i; \sigma_i\} = S\left(\sum_i q_i \sigma_i\right) - \sum_i q_i S(\sigma_i)$. To calculate the amount of quantum correlation, Alice projects her system onto another basis $\left\{\left|a_i^2\right\rangle\right\}$ that is mutually unbiased to the optimum basis $\left\{\left|i\rangle\right\}$ for classical correlation. From $\left|\left\langle i|a_i^2\right\rangle\right|^2 = \frac{1}{d_1}$, we have

$$\left\langle a_j^2 | \rho^{cq} | a_j^2 \right\rangle = \sum_i q_i \left\langle a_j^2 | (|i\rangle \langle i|) | a_j^2 \right\rangle \sigma_i$$

$$= \frac{1}{d_A} \sum_i q_i \sigma_i = \frac{1}{d_A} \rho_B.$$

$$(7)$$

For each different result *j* that Alice obtains, Bob is left with the same state $\rho_B = \sum_i q_i \sigma_i$; thus, Bob's state has no correlation with Alice's result, and we immediately have $Q_2 = Q_3 \cdots = 0$ according to the definitions of these quantities. Hence, for a CQ state, the correlation vector is given as $\vec{C} = (C_1, 0, \dots, 0)$. The only correlation present in a CQ state is the classical correlation, and the quantum correlation in any MUB vanishes!

Next, we consider the Werner states of a $d \times d$ dimensional system³⁵,

$$\rho_w = \frac{1}{d(d-\alpha)} (I - \alpha P), \qquad (8)$$

where $-1 \le \alpha \le 1$, *I* is the identity operator in the d^2 -dimensional Hilbert space, and $P = \sum_{i,j=1}^{d} |i\rangle \langle j| \otimes |j\rangle \langle i|$ is the operator that exchanges A and B. Because the Werner states are invariant under a unitary transformation of the form $U \otimes U$, the maximal classical correlation can be revealed when Alice simply projects her system onto the basis states { $|i\rangle$ }. With probability $p_i = \frac{1}{d}$, Alice will obtain the *i*-th basis state $|i\rangle_i$ and Bob will be left with the state $\rho_i^B = A \langle i | \rho_{AB} | i \rangle_A / p_i = \frac{1}{d - \alpha} (I - \alpha | i \rangle \langle i |).$ It is straightforward to show that $C_1 = \chi \{ p_i; \rho_i^B \} = \log_2 \left(\frac{d}{d-\alpha} \right) + \frac{1-\alpha}{d-\alpha} \log_2(1-\alpha) \equiv \chi_w.$ Due to the symmetry of the Werner states, it is not difficult to demonstrate that $Q_2 = Q_3 = \cdots = C_1 = \chi_w$. Therefore, for the Werner state ρ_w , the correlation vector is given by $\vec{C} = (\chi_w, \chi_w, \dots, \chi_w)$. The maximal quantum correlation in a Werner state can be revealed in any basis, and it is equal to the maximal classical correlation C_1 . However, the correlation vector of a Werner state is different from that of a pure state because $C_1 \leq S(\rho_B) = \log_2 d$. The inequality becomes an equality only when d = 2 and $\alpha = 1$, in which case, the Werner state becomes a pure state $\rho_w = |EPR\rangle \langle EPR|$. For the Werner states, the symmetric discord is equal to the quantum discord D¹² when Alice's measurement is restricted to projective mea-



Figure 3 | Three measures of quantum correlation for the Werner states as functions of α when d = 2 (left) and d = 3 (right). The red curve represents our measure Q_2 , the green curve represents the quantum discord D and the blue curve represents the entanglement of formation E_{f} .

surements. The entanglement of formation E_f for the Werner states is

given as
$$E_f(\rho_w) = h\left(\frac{1}{2}\left(1 + \sqrt{1 - \left[\max\left(0, \frac{d\alpha - 1}{d - \alpha}\right)\right]^2}\right)\right)$$
, with $h(\alpha) = -\alpha \log \alpha = -(1 - \alpha)\log(1 - \alpha)^{36}$. The three different

 $h(x) \equiv -x \log_2 x - (1 - x) \log_2(1 - x)^{36}$. The three different measures of quantum correlation, i.e., our measure of maximal quantum correlation Q_2 , the quantum discord D and the entanglement of formation, are illustrated in Fig. 3 for comparison. From this figure, we see that the curve for entanglement of formation intersects the other two curves; thus, E_f can be larger or smaller than Q_2 (D).

As the last example, we consider a family of two-qubit states, where the reduced density matrices of both qubits are proportional to the identity operator. Such a state can be written in terms of Pauli matrices,

$$\rho_{AB} = \frac{1}{4} \left(I_2 \otimes I_2 + \sum_{j,k=1}^3 w_{jk} \sigma_j \otimes \sigma_k \right), \tag{9}$$

where I_2 is the identity operator in the two-dimensional Hilbert space of a qubit, and w_{jk} are real numbers that satisfy certain conditions to ensure the positivity of the matrix in (9). These two-qubit states can be transformed by a local unitary transformation (that does not change the correlations) to the following form:

$$\sigma_{AB} = \frac{1}{4} \left(I_2 \otimes I_2 + \sum_{j=1}^3 r_j \sigma_j \otimes \sigma_j \right)$$
(10)

which is equivalent to the Bell-diagonal states. To ensure the positivity of the matrix in (10), the real vector $\vec{r} = (r_1, r_2, r_3)$ must lie inside or on the boundary of the regular tetrahedron that is the convex hull of the four points: (-1, -1, -1), (-1, 1, 1), (1, -1, 1) and (1, 1, -1) (which are the four Bell states). The singular values of the matrix w_{jk} are given by $|r_j|$. We rearrange the three numbers $\{r_1, r_2, r_3\}$ according to their absolute values and denote the rearranged set as $\{\bar{r}_1, \bar{r}_2, \bar{r}_3\}$ such that $|\bar{r}_1| \ge |\bar{r}_2| \ge |\bar{r}_3|$.

In the Methods, we prove that the correlation vector of the state in

(9) is given by
$$\vec{C} = (\chi_1, \chi_2, \chi_3)$$
, where $\chi_j = 1 - h\left(\frac{1 + |\vec{r}_j|}{2}\right)$ with $h(x) \equiv$

 $\begin{aligned} -x \log_2 x - (1-x) \log_2(1-x). \text{ To have some intuition of this result,} \\ \text{we consider some special classes of states with only one parameter.} \\ \text{When } r_1 = r_2 = r_3 = -\frac{\alpha}{2-\alpha} \text{ with } -1 \leq \alpha \leq 1 \text{, the states in (10)} \\ \text{become the Werner states for } d = 2 \text{ in (6). When } r_1 = r_2 = 1 - 2p \text{ and } r_3 = -1 \text{ with } 0 \leq p \leq 1 \text{, the states in (10) become } \rho_1 = p |\psi^-\rangle \\ \langle \psi^-| + (1-p) |\psi^+\rangle \langle \psi^+| \text{; we obtain } C_1 = 1 \text{ and } Q_2 = Q_3 = 1 - h(p). \\ \text{When } r_1 = 1 - 2p \text{ and } r_2 = r_3 = -p \text{, the states in (10) become} \\ \rho_2 = p |\psi^-\rangle \langle \psi^-| + \frac{1-p}{2} \left(|\psi^+\rangle \langle \psi^+| + |\phi^+\rangle \langle \phi^+| \right) \text{; we have } C_1 = max \left\{ 1 - h(p), 1 - h\left(\frac{1+p}{2}\right) \right\}, \quad Q_2 = 1 - h\left(\frac{1+p}{2}\right) \text{ and } Q_3 = min \\ \left\{ 1 - h(p), 1 - h\left(\frac{1+p}{2}\right) \right\}. \text{ Here, } |\psi^-\rangle = |EPR\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle), \\ |\psi^+\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \text{ and } |\phi^+\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle). \text{ Our measure of quantum correlation } Q_2 \text{ is compared with the quantum dis-} \end{aligned}$

sure of quantum correlation Q_2 is compared with the quantum discord D and the entanglement of formation E_f for ρ_1 and ρ_2 in Fig. 4.

Inequality relations between correlation measures. It is not difficult to show that the relation $Q_2 \leq D$ holds for the Werner states, and for all the example states considered in this article. However, it is not clear whether this inequality holds for any bipartite states. If $Q_2 \leq D$ holds for any bipartite states, then one can easily have $C_1 + Q_2 \leq S(A:B)$ where $S(A:B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$ denotes the quantum mutual information.

Nevertheless, we can prove the following inequality:

$$C_1 + Q_2 \le H_1 + H_2 + S(\rho_B) - S(\rho_{AB}) - \log_2 d_A \tag{11}$$

where H_{γ} ($\gamma = 1, 2$) denotes the Shannon entropy of the probability distribution $\left\{p_{i}^{(\gamma)}\right\}$ obtained by the measurement on system A in the basis $\left\{|\mathcal{A}_{i}^{\gamma}\rangle_{A}|i=1,\cdots,d_{A}\right\}$. The proof is given in the Methods. Since $H_{\gamma} \leq \log_{2} d_{A}$, one immediately has

$$C_1 + Q_2 \le S(\rho_B) - S(\rho_{AB}) + \log_2 d_A.$$
(12)

As C_1 and Q_2 are the two largest elements in the correlation vector, when they are replaced by correlations in any two MUBs, inequalities (11) and (12) still hold.



Figure 4 | Different measures of quantum correlation for two special classes of states: $\rho_1 = p |\psi^-\rangle \langle \psi^-| + (1 - p) |\psi^+\rangle \langle \psi^+|$ (left) and $\rho_2 = p |\psi^-\rangle \langle \psi^-| + \frac{1-p}{2} (|\psi^+\rangle \langle \psi^+| + |\phi^+\rangle \langle \phi^+|)$ (right). In each figure, the red curve represents our measure Q_2 , the green curve represents the quantum discord *D*, and the blue curve represents the entanglement of formation E_f In the left figure, the green curve is not shown because $D = Q_2$ for ρ_1 .

Discussion

Our measures of quantum correlation provide a natural way to quantify the "spooky action at a distance", and directly reveal the essential feature of the genuine quantum correlation, i.e., the simultaneous existence of correlations in complementary bases. This feature enables quantum key distribution with entangled states, since the quantum correlation that exists simultaneously in two (k) MUBs, which is quantified by Q_2 (Q_k), is the resource for entanglement-based QKD via two (k) MUBs. Quantitative relation between the genuine quantum correlation and the secret key fraction in QKD could be studied in further work.

All the measures considered above are not symmetric with respect to the exchange of systems A and B, as only system A's bases are considered to reveal the correlation. Symmetric measures and a symmetric correlation vector are also introduced and discussed in the Methods. A further study of the relation between the symmetric correlation vector and the symmetric discord¹² could reveal the difference between these measures in practical applications.

There are some open questions. Are our measures (Q_2, Q_3) of genuine quantum correlation additive? How do they behave under some natural operations (for example, Alice adds an ancilla)? Do our measures (Q_2, Q_3) behave like the entanglement measures that do not increase under local operations and classical communication (LOCC)⁹, or more like the measures of nonclassical correlation beyond entanglement (for example, quantum discord) that could increase under LOCC³⁸? We hope that further investigations will unveil these mysteries.

Methods

Proof of the inequality (11). Here we prove inequality (11) in the main text. Let $\{p_i^{(\gamma)}\}(\gamma = 1,2)$ denote the probability distribution obtained by the

measurement on system A in the basis $\{|\mathcal{A}_i^{\gamma}\rangle_A|i=1,\cdots,d_A\}$, i.e., $p_i^{(\gamma)} = tr_{AB}$ $((|\mathcal{A}_i^{\gamma}\rangle\langle\mathcal{A}_i^{\gamma}|\otimes I)\rho_{AB})$. Let $H_{\gamma}(\gamma = 1, 2)$ denote the Shannon entropy of the probability distribution, $H_{\gamma} = \sum_{i=1}^{d_A} -p_i^{(\gamma)}\log_2 p_i^{(\gamma)}$. Here, the basis $\{|\mathcal{A}_i^1\rangle_A|i=1,\cdots,d_A\}$ is the optimum basis for measurement on system A to achieve the maximum classical correlation C_1 , and the basis $\{|\mathcal{A}_i^2\rangle_A\}$ is the optimum basis to achieve Q_2 among the bases that are mutually unbiased to $\{|\mathcal{A}_i^1\rangle_A\}$. However, the proof below only requires that $\{|\mathcal{A}_i^2\rangle_A\}$ and $\{|\mathcal{A}_i^2\rangle_A\}$ are mutually unbiased to each other.

Let $\rho^{(\gamma)} = \sum_{i=1}^{d_A} |\mathcal{A}_i^{\gamma}\rangle \langle \mathcal{A}_i^{\gamma}| \otimes p_i^{(\gamma)} \rho_i^{(\gamma)}$ with $\gamma = 1, 2$, where $\rho_i^{(\gamma)} = \langle \mathcal{A}_i^{\gamma}| \rho_{AB} |\mathcal{A}_i^{\gamma}\rangle / p_i^{(\gamma)}$.

The uncertainty relation³⁷ gives

$$S(\{|\mathcal{A}_i^1\rangle\}|B) + S(\{|\mathcal{A}_i^2\rangle\}|B) \ge \log_2 d_A + S(A|B)$$
(13)

where $S(A|B) = S(\rho_{AB}) - S(\rho_B)$, and $S(|\mathcal{A}_i^{\gamma}\rangle|B) = S(\rho^{(\gamma)}) - S(\rho_B)(\gamma = 1, 2)$. As $\rho^{(\gamma)}$ is a CQ state, one can show that $S(\rho^{(\gamma)}) = H_{\gamma} + \sum_i p_i^{(\gamma)} S(\rho_i^{(\gamma)})$. Therefore,

$$H_{1} + \sum_{i} p_{i}^{(1)} S(\rho_{i}^{(1)}) - S(\rho_{B})$$

+ $H_{2} + \sum_{i} p_{i}^{(2)} S(\rho_{i}^{(2)}) - S(\rho_{B})$
 $\geq \log_{2} d_{A} + S(\rho_{AB}) - S(\rho_{B})$ (14)

As $C_1 = S(\rho_B) - \sum_i p_i^{(1)} S(\rho_i^{(1)})$ and $Q_2 = S(\rho_B) - \sum_i p_i^{(2)} S(\rho_i^{(2)})$, we immediately have

$$C_1 + Q_2 \le H_1 + H_2 + S(\rho_B) - S(\rho_{AB}) - \log_2 d_A$$
(15)

which completes the proof of the inequality.

Calculation of the correlation vector for the states in (9). In this paragraph, we shall demonstrate that the correlation vector of the state in (9) is given by $\vec{C} = (\chi_1, \chi_2, \chi_3)$, where $\chi_j = 1 - h\left(\frac{1 + |\vec{r}_j|}{2}\right)$ with $h(x) \equiv -x \log_2 x - (1 - x) \log_2(1 - x)$. We perform the calculation in the transformed basis, with the states rewritten in Eq. (10). Without loss of generality, we can suppose the numbers r_j are already arranged according to $|r_1| \ge |r_2| \ge |r_3|$; then, we only need to prove that $\vec{C} = (\chi_1, \chi_2, \chi_3)$, where

 $\chi_j = 1 - h\left(\frac{1 + |r_j|}{2}\right)$. A projective measurement performed on qubit A can be written $P_+^A = \frac{1}{2}(I_2 \pm \vec{n}\cdot\vec{\sigma})$, parameterized by the unit vector \vec{n} . We have

$$p \pm \rho_{\pm}^{B} \equiv Tr_{A} \left(P_{\pm}^{A} \rho_{AB} \right) = \frac{1}{2} \cdot \frac{1}{2} \left(I_{2} \pm \sum_{j} n_{j} r_{j} \sigma_{j} \right).$$
(16)

When Alice obtains \pm , qubit B will be in the corresponding states $\rho_{\pm}^{B} = \frac{1}{2} \left(I_{2} + \sum_{j} n_{j} r_{j} \sigma_{j} \right)$, each occurring with probability $\frac{1}{2}$. The entropy $S(\rho_{\pm}^{B})$ reaches its minimum value $h\left(\frac{1+|r_{1}|}{2}\right)$ when $\vec{n} = (1,0,0)$. From $\rho_{B} = p + \rho_{\pm}^{B} + p - \rho_{-}^{B} = \frac{1}{2}I_{2}$ and $S(\rho_{B}) = 1$, we immediately have $C_{1} = 1 - h\left(\frac{1+|r_{1}|}{2}\right)$. The basis for Alice's projection $P_{\pm}^{A} = \frac{1}{2}(I_{2} + \vec{n}'\cdot\vec{\sigma})$ in the definition of Q_{2} must be mutually unbiased to the basis parameterized by $\vec{n} = (1,0,0)$; therefore, the unit vector \vec{n}' must be in the form $\vec{n}' = (0,n_{2},n_{3})$. The maximum in the definition of Q_{2} is reached when $\vec{n}' = (0,1,0)$, and thus a calculation similar to that for C_{1} yields $Q_{2} = 1 - h\left(\frac{1+|r_{2}|}{2}\right)$. For a qubit system, three MUBs exist. We can reveal the quantum correlation in another (the last) MUB, which corresponds to the case $\vec{n}'' = (0,0,1)$. We easily obtain $Q_{3} = 1 - h\left(\frac{1+|r_{3}|}{2}\right)$. For the general case in which the numbers r_{j} do not follow $|r_{1}| \geq |r_{2}| \geq |r_{3}|$, a similar argument yields $\vec{C} = (\chi_{1}, \chi_{2}, \chi_{3})$ with $\chi_{j} = 1 - h\left(\frac{1+|\vec{r}_{j}|}{2}\right)$.

Symmetric correlation vector. The correlation vector defined in the main text relies on a special choice of the measure of classical correlation; it is not symmetric with respect to exchange of A and B. Here, we consider an alternative definition of the correlation vector, which is symmetric with respect to the exchange of A and B.

For any bipartite quantum state ρ_{AB} , Alice chooses a basis $\{|a_i\rangle_A|i=1,\cdots,d_A\}$ of her system in a d_A -dimensional Hilbert space and Bob chooses a basis $\{|b_i\rangle_A|i=1,\cdots,d_B\}$ of his system in a d_B -dimensional Hilbert space, and each one performs a measurement projecting his/her system onto the corresponding basis states. With probability $p_{ij} = tr_{AB} \left(\left(|a_i\rangle_A \langle a_i| \otimes |b_j\rangle_A \langle b_j | \right) \rho_{AB} \right)$, Alice and Bob will obtain the *i*-th and *j*-th results, respectively. The correlation of their measurement results is well characterized by the classical mutual information:

$$I\{p_{ij}\} = H\{p_i^a\} + H\{p_j^b\} - H\{p_{ij}\}, \qquad (17)$$

where $H \{p_k\}$ is the Shannon entropy of the probability distribution $\{p_k\}$, and $p_i^a = \sum_i p_{ij}$ and $p_j^b = \sum_i p_{ij}$ are the marginal probability distributions. In other words, $H\{p_i^a\} = \sum_i -p_i^a \log_2 p_i^a$, and $H\{p_{ij}\} = \sum_{ij} -p_{ij} \log_2 p_{ij}$.

The symmetric measure of classical correlation C_1^c in the state ρ_{AB} is defined as the maximal classical mutual information of the local measurement results, maximized over all local bases for both sides, i.e.,

$$C_1^s(\rho_{AB}) = \max_{\left\{|a_i\rangle \otimes |b_j\rangle\right\}} I\left\{p_{ij}\right\}.$$
(18)

The symmetric measure of classical correlation was discussed in¹² (where the notation I_{max} was used). A product basis $\left\{ |a_i^1\rangle \otimes |b_j^1\rangle | i=1, \cdots, d_{A,j}=1, \cdots, d_B \right\}$ that achieves the maximum in (18) is called a C_1^s -basis, and is denoted as $\left\{ |\mathcal{A}_i^1\rangle \otimes |\mathcal{B}_j^1\rangle | i=1, \cdots, d_{A,j}=1, \cdots, d_B \right\}$.

The symmetric measure of maximal quantum correlation Q_2^s is defined as the maximal residual correlation over all local bases that are mutually unbiased to a C_1^s -bases $\left\{ \left| \mathcal{A}_i^1 \right\rangle \otimes \left| \mathcal{B}_j^1 \right\rangle \right\}$, further maximized over all possible C_1^s -bases (if not unique), i.e.,

$$Q_{2}^{s}(\rho_{AB}) = \max_{\left\{ \left| \mathcal{A}_{i}^{1} \right\rangle \otimes \left| \mathcal{B}_{j}^{1} \right\rangle \right\}} \max_{\left\{ \left| a_{i}^{2} \right\rangle \otimes \left| b_{j}^{2} \right\rangle \right\}} I\left\{ p_{ij}^{\prime} \right\},$$
(19)

where $\{|a_i^2\rangle\}\left(\left\{|b_j^2\rangle\right\}\right)$ is mutually unbiased to $\{|\mathcal{A}_i^1\rangle_A\}\left(\left\{|\mathcal{B}_j^1\rangle_B\right\}\right)$ and $p'_{ij} = tr_{AB}\left(\left(|a_i^2\rangle_A\langle a_i^2|\otimes |b_j^2\rangle_A\langle b_j^2|\right)\rho_{AB}\right)$. A basis $\{|a_i^2\rangle\otimes |b_j^2\rangle\}$ that achieves the maximum in (19) is called a Q_2^s -basis, and is denoted as $\{|\mathcal{A}_i^2\rangle\otimes |\mathcal{B}_j^2\rangle\}$. We redefine the C_1^s -bases $\{|\mathcal{A}_i^1\rangle\otimes |\mathcal{B}_j^1\rangle\}$ as the bases that achieve the maximum in (18) as well as the maximum in (19).

Similarly, Q_3^s denotes the residual quantum correlation in a third complementary basis that is mutually unbiased to both $\left\{ |\mathcal{A}_i^1\rangle \otimes |\mathcal{B}_j^1\rangle \right\}$ and $\left\{ |\mathcal{A}_i^2\rangle \otimes |\mathcal{B}_j^2\rangle \right\}$. In this



manner, we have an alternative correlation vector $\vec{C}_s = (C_1^s, Q_2^s, Q_3^s, \cdots, Q_M^s)$, which is symmetric with respect to the change of A and B.

Because the Holevo bound is an upper bound of accessible classical mutual information, we immediately know from the above definitions that the asymmetric correlation vector \vec{C} is an upper bound of the symmetric correlation vector \vec{C}_s for each component, i.e., $C_1 \ge C_1^s$, $Q_2 \ge Q_2^s$, \cdots , $Q_M \ge Q_M^s$. It is not difficult to demonstrate that the asymmetric correlation vector \vec{C} actually coincides with the symmetric correlation vector \vec{C}_s (i.e., $\vec{C} = \vec{C}_s$) for the CQ states, the Werner states and the two-qubit states in Eq. (9).

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Author contributions

S.W. introduced the idea and definitions, calculated the examples and wrote the manuscript. S.Y. proved the inequalities relations. Z.M. and Z.C. preformed analyses and discussed the results. All authors reviewed the manuscript.

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