Complementarity and correlations

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We investigate the relation between complementary properties and correlations of composite quantum systems. We introduce three measures of correlations which are based on local measurements in complementary bases. These measures are linked to the mutual information, the Pearson correlation coefficient and the sum of conditional probabilities, respectively. We show that states which have complementary correlations beyond a certain threshold must be entangled. The reverse is not true, however. We also show that, surprisingly, states with non-zero quantum correlations may have less correlations on complementary observables than classically correlated states.

Two properties of a quantum state are called complementary if they are such that, if one knows the value of one property, all possible values of the other property are equiprobable. More rigorously, let \(|a_i\rangle\) represent the eigenstates corresponding to possible values of a nondegenerate property \(A = \sum_i f(a_i)|a_i\rangle\langle a_i|\), and \(|c_j\rangle\) the eigenstates of a nondegenerate property \(C = \sum_j g(c_j)|c_j\rangle\langle c_j|\) (with \(f\) and \(g\) arbitrary bijective functions). Then \(A\) and \(B\) are complementary properties if for all \(i, j\) we have \(|\langle a_i|c_j\rangle|^2 = 1/d\), \(d\) being the Hilbert space dimension. Clearly complementary properties with this definition identify two mutually unbiased bases (MUBs) \(\{|a_i\rangle\}_{i=1}^d\). Here we study what correlations in measurements of these complementary properties tell us about the quantum correlations of the state of the system.

Typically one discusses entanglement \(\mathcal{E}\) and discord \(\mathcal{D}\) in terms of non-locality, Bell inequality violations, monotones over LOCC, etc. For example, previous literature on entanglement focused on time-reversal (for the PPT criterion \(\mathcal{E}\)), local uncertainty relations \(\mathcal{U}\), entropic uncertainty relations \(\mathcal{U}_e\), entanglement witnesses \(\mathcal{W}\), concurrence \(\mathcal{C}\), the cross-norm criterion \(\mathcal{C}_X\) and the covariance matrix criterion \(\mathcal{C}_C\) (the latter encompassing many of the former).

Literature on quantum correlations focused mostly on information-theoretic arguments \(\mathcal{I}\). All these proposals are inequivalent to the analysis proposed here, since our method is based on correlations among two complementary properties (and can be easily extended to more). In \(\mathcal{I}\) related approaches using specific measures of correlations (different from the ones used here) were proposed.

The outline of the paper follows. We start by describing the general scenario we employ for correlation evaluation. We then introduce different measures of correlations and state our results and our conjectures regarding entanglement and discord. We provide some examples of applications. The details of the proofs of our results are reported in the appendix.

**Complementary correlations:** — Consider two systems of finite dimension \(d_1\) and two observables \(A \otimes B\) and \(C \otimes D\) (Fig. 1) where \(A\) and \(C\) are complementary on the first system (namely \(|a_i|c_j\rangle = 1/\sqrt{d}\) for all eigenstates of \(A\) and \(C\)) and \(B\) and \(D\) on the second. For example, take the computational basis of the two systems as the eigenstates of \(A\) and \(B\), and the Fourier basis as the ones of \(C\) and \(D\). We can quantify the correlations between the results of measurements of \(A\) and \(B\) with some correlation measure \(\mathcal{X}_{AB}\) and the correlations between \(C\) and \(D\) with \(\mathcal{X}_{CD}\). As \(\mathcal{X}\) below we will define and investigate three possibilities: the mutual information \(\mathcal{X}_{XY} = I_{XY}\), the sum of conditional probabilities \(\mathcal{X}_{XY} = \mathcal{S}_{XY}\), and the Pearson correlation coefficient \(\mathcal{X}_{XY} = \mathcal{C}_{XY}\). A measure of the overall correlation of the initial state, the “complementary correlations”, can then be given as the sum of the absolute value of the two measures \(|\mathcal{X}_{AB}| + |\mathcal{X}_{CD}|\) or as the product \(|\mathcal{X}_{AB}\mathcal{X}_{CD}|\). The latter is typically a weaker measure than the former, since an upper bound for the sum implies an upper bound for the product. Indeed, \((|\mathcal{X}_{AB}|^2 + |\mathcal{X}_{CD}|^2)^2 \geq 0\) implies \(2|\mathcal{X}_{AB}\mathcal{X}_{CD}| \leq |\mathcal{X}_{AB}| + |\mathcal{X}_{CD}|\). Thus we will mainly consider the sum of correlations on complementary observables \(|\mathcal{X}_{AB}| + |\mathcal{X}_{CD}|\) as a way to evaluate the com-

\(^1\) Many results can be immediately extended to the case where the two systems have different dimensions.
plimentary correlations. [One could also consider more than two complementary variables, by adding MUBs.]

**Mutual Information:** We start considering the mutual information:

\[ I_{AB} = H(A) - H(A|B), \]

where \( H(A) \) is the Shannon entropy of the probabilities of the measurement outcomes of the first system and \( H(A|B) \) is the conditional entropy of the outcomes of the first conditioned on the second. The complementary correlations are then \( I_{AB} + I_{CD} \).

The relation of this quantity to the entanglement and the discord of the state of the system is illustrated by the following results: (i) The state of a bipartite composite quantum system is maximally entangled if and only if there exist two complementary measurement bases where \( I_{AB} + I_{CD} = 2 \log_2 d \); (ii) If \( I_{AB} + I_{CD} > \log_2 d \), the state of the bipartite system is entangled; (iii) The separable states that satisfy this inequality with equality (i.e. \( I_{AB} + I_{CD} = \log_2 d \)) are the classically-correlated (CC) zero-discord states of the form

\[ \rho_{cc} = \sum_i |a_i\rangle\langle a_i| \otimes |b_i\rangle\langle b_i|/d \]

with \( |a_i\rangle \) and \( |b_i\rangle \) eigenstates of \( A \) and \( B \) (or the analogous state with a uniform convex combination of eigenstates of \( C \) and \( D \)). Some examples of \( I_{AB} + I_{CD} \) for various families of states are plotted in Fig. 2a, where we emphasize the threshold \( \log_2 d \) above which all states are entangled.

The first result follows from the fact that each term in the sum is upper bounded by \( \log_2 d \) by definition. The maximum value for the sum is then \( 2 \log_2 d \) and is achievable if and only if there is maximal correlation both between \( A \) and \( B \), and between \( C \) and \( D \). Simple properties of the conditional probabilities (see Appendix) imply that this can happen for a suitable choice of observables if and only if the state is maximally entangled. The second result is a consequence of the concavity of the entropy and of Maassen and Uffink’s entropic uncertainty relation [21] (see Appendix for the details). It gives a sufficient condition for entanglement that can be used for entanglement detection. The third result is surprising: one might expect that the separable states at the boundary with the entangled region are highly quantum correlated, whereas we find that they only have classical correlations (CC) and no discord. This means that quantum correlated states without entanglement do not have higher correlations on complementary properties than CC states. This result is peculiar for the mutual information as a figure of merit, it is no longer true for the Pearson correlation (where a family of QQ states sits on the border, as shown in Fig. 2b). It can be proved by analyzing the conditions for equality of the concavity of the entropy and of Maassen and Uffink’s inequality (see Appendix).

**Pearson correlation:** The second measure of correlation we consider is the Pearson correlation coefficient \( C_{AB} \),

\[ C_{AB} = \frac{\langle AB \rangle - \langle A \rangle \langle B \rangle}{\sigma_A \sigma_B}, \]

where, as before, \( A \) and \( B \) denote observables relative to the two systems, \( \{X\} = Tr[X\rho] \) is the expectation value on the quantum state \( \rho \) and \( \sigma_X^2 \) is the variance of the observable \( X \). In contrast to the classical Pearson correlation coefficient, the quantum one is, in general, complex if \( A \) and \( B \) do not commute, but as in the classical case, its modulus is upper-bounded by one:

\[ |\langle AB \rangle - \langle A \rangle \langle B \rangle|^2 = \frac{1}{2} \left( |\{A,B\}|^2 - \langle A \rangle \langle B \rangle \right)^2 =\]

\[ |\frac{1}{2} \{\langle A,B \rangle\}^2 + \frac{1}{2} \{\langle A \rangle - \langle B \rangle \}|^2 \leq \sigma_A^2 \sigma_B^2, \]

where \[|\cdot| \} and \{\cdot,\cdot\} denote the commutator and anti-commutator respectively, and where the final inequality

\[ \leq \frac{1}{2} \left( \frac{1}{2} \{\langle A,B \rangle\}^2 + \frac{1}{2} \{\langle A \rangle - \langle B \rangle \}|^2 \right) \leq \sigma_A^2 \sigma_B^2. \]
is the Schrödinger uncertainty relation \[23\].

We now use \(|C_{AB}| + |C_{CD}|\) as a measure of complementary correlations to recover some entanglement properties of the system state. The Pearson coefficient gauges only the linear correlation of two stochastic variables, so it will not detect maximal correlation even for a maximally entangled state unless pairs of observables are linear in each other’s eigenvalues (e.g., it would fail if \(A = \sum_j j|j\rangle\langle j|\) and \(B = A^\dagger\)). However, if one restricts to linear observables, one can prove that a state is maximally entangled if and only if there exist two complementary bases such that \(|C_{AB}| + |C_{CD}| = 2d\), e.g., if one uses \(A = B = \sum_j j|j\rangle\langle j|\), \(C = D = \sum_j j|f_j\rangle\langle f_j|\) where \(|j\rangle\) and \(|f_j\rangle\) are the two complementary bases. The proof follows from the properties of the conditional probabilities (used to prove the analogous statement for the mutual information) and from the fact that the Pearson coefficient is \pm 1\) if and only if there is a functional relation that connects the two stochastic variables (details in Appendix).

Instead, for non maximally entangled states we have two conjectures which are supported by numerical evidence: (i) If \(|C_{AB}| + |C_{CD}| > 1\), the two systems are entangled. As for the mutual information, the inequality is tight since \(\rho_{cc}\) is separable and has \(|C_{AB}| + |C_{CD}| = 1\;\); (ii) If \(|C_{AB}| + |C_{CD}| > 1/4\), the two systems are entangled. Also this inequality is tight: it is attained by the separable state \(\sum_j (|a_i a_i\rangle + |c_i c_i\rangle)/2d\), with \(|c_i\rangle\) eigenstates of \(C\). As argued above, the conjecture with the product is weaker than the one with the sum: proving that all separable states have \(|C_{AB}| + |C_{CD}| \leq 1\) implies \(|C_{AB} C_{CD}| \leq 1/4\).

The proof of these conjectures is complicated by the fact that the convexity properties of \(C_{AB}\) is unknown. Nonetheless, they are natural conjectures that are easy to verify for large classes of states (e.g., see Fig. [3]). We have also performed extensive numerical checks by testing them on large sets of random states generated according to the prescription described in [23], and verifying that no state with non-positive partial transpose [4] lies over the conjectured threshold. The Pearson correlation only measures linear correlation, whereas the mutual information measures all types of correlations. So one could think that the latter is stronger and that these conjectures are implied by the mutual information results of the previous section. Surprisingly, this is false since there exist probability distributions that have maximal Pearson correlation but negligible mutual information [24]. Indeed, consider the family of entangled two-qubit states

\[
|\psi_\epsilon\rangle = \epsilon|00\rangle + \sqrt{1 - \epsilon^2}|11\rangle \quad (5)
\]

with \(\epsilon \in [0, 1]\). If one uses \(A = B = |1\rangle\langle 1|\) and \(C = D = |+\rangle\langle +|\), for all \(\epsilon > 0\) such state has \(|C_{AB}| + |C_{CD}| = 1 + 2\epsilon \sqrt{1 - \epsilon^2} > 1^2\), but \(|\psi_\epsilon\rangle\) clearly has negligible mutual information for \(\epsilon \to 0\). In other words, the Pearson correlation identifies \(|\psi_\epsilon\rangle\) as entangled for all \(\epsilon > 0\) (assuming the above conjectures), whereas \(\rho_{cc}\) does not even identify it as classically correlated at all for \(\epsilon \to 0\). Indeed, numerical simulations suggest that Pearson correlation is more effective at detecting entanglement in random states than mutual information.

**Sum of conditional probabilities:** The third measure of correlation we consider is the sum of conditional probabilities \(S_{AB}\), defined as

\[
S_{AB} = \sum_i p(a_i|b_i) \quad (6)
\]

where \(p(a_i|b_i)\) is the probability of outcome \(a_i\) on the first system conditioned on result \(b_i\) on the second. [This is a somewhat limited measure of correlations as the correspondence \(a_i \leftrightarrow b_i\) among results is clearly arbitrary. A more relevant measure of correlation should also maximize (or minimize) over the permutations of the measurement outcomes, but for the sake of simplicity we will avoid it.] In [23] a similar approach was used, but employing joint probabilities in place of conditional ones.

Gauging complementary correlations with the sum \(S_{AB} + S_{CD}\) we can again obtain information about entanglement and discord: (i) Analogously to the case of the mutual information, the sum is optimized only for maximally entangled states: a state is maximally entangled if and only if there exist two complementary bases such that \(S_{AB} + S_{CD} = 2d\); (ii) As for the Pearson correlation, we have a conjecture for non-maximally entangled states: if \(S_{AB} + S_{CD}\) has a value outside the interval \([1, d + 1]\), we conjecture that the two systems are entangled. As in the previous cases, the inequalities are tight since the upper bound is attained by the separable state \(\rho_{cc}\) and the lower bound by the separable state \(\sum_i |a_i b_i\rangle\langle a_i b_i|\)/\(d\), with \(\oplus\) sum modulo \(d\).

Let us analyse the case of separable states. We remind the reader that classical-quantum (CQ) and quantum-classical (QC) states have the form \(\sum_i p_i|a_i\rangle\langle a_i| \otimes |\rho_i\rangle\) and \(\sum_i p_i|a_i\rangle \otimes |\rho_i\rangle\), respectively, where \(\{\rho_i\}\) is a set of orthogonal states for one subsystem and \(\{a_i\}\) is not an orthogonal set of states. Note that separable quantum-quantum (QQ) states comprise all separable ones that are not CC, CQ or QC.

For these states we can prove that: (iii) if CC states have maximal correlations on one of two complementary variables, they are uncorrelated on the other [formally: if \(p(a_i|b_i) = 1\) \(\forall i\) then we must have \(p(c_i|d_i) = 0\)].
1/d ∀i, where \(a_i, b_i, c_i, d_i\) are the results of the measurements of \(A, B, C, D\) with \(A\) complementary to \(C\) and \(B\) to \(D\); (iv) CQ states cannot have maximal correlations on any variable [formally: we cannot obtain \(p(a_i|b_i) = 1\ ∀i\), even when \(p(c_i|d_i) = 1/d\)]; (v) QQ states can have only partial correlation on complementary properties. For example, the separable two-qubit state \(|00⟩ + |11⟩|+⟩|+⟩|+⟩|−⟩|−⟩|−⟩|−⟩|−⟩|−⟩|−⟩⟩/4 has partial correlation on both complementary variables, since \(p(00) = p(11) = p(+|+) = p(−|−) = 3/4\).

Given the properties (iii) and (iv), one might suspect that separable states with non vanishing quantum correlations have always less correlations on complementary properties, but this is not the case, as emphasized by (v). Summarizing, CC states can have maximal correlation only on one property, CQ states cannot have maximal correlation in any property, and QQ states can have some correlation on multiple properties, but you need pure, maximally entangled states to get maximal correlations on more than one property.

Regarding the result (i), the proof is a direct consequence of simple properties of conditional probabilities (see Appendix) as for the cases seen previously. The difficulty in proving the conjecture (ii) stems again from a lack of definite concavity properties of \(S_{AB}\), but as for the previous conjecture we have extensively tested it numerically on random states. One may ask whether the sum over all outcomes in the statement of the conjecture is necessary. Indeed it is: the statement that all separable states satisfy \(1/d ≤ p(a_i|b_i) + p(c_i|d_i) ≤ 1 + 1/d\) for some \(i\) is false (where the two bounds \(1/d\) and \(1 + 1/d\) give the bounds \(1\) and \(d + 1\) we used above when the sum over \(i\) is performed). A counterexample is the separable state \(|00⟩ + |11⟩|+⟩|+⟩⟩/2\) of two qubits for which \(p(00) + p(+|+) = 5/3\). If one uses joint probabilities in place of conditional ones, a sufficient condition for entanglement can indeed be proven [2]. The results (iii) and (iv) can be proved at the same time by using simple properties of CC and CQ states when they are expressed in two complementary bases (see Appendix), whereas property (v) is a direct consequence of the example provided above.

Conclusions:— In the previous sections we provided sufficient conditions for entanglement using the mutual information and we have conjectured sufficient conditions using the Pearson correlation and the sum of conditional probabilities. One can ask if it is possible to give necessary and sufficient conditions based on correlations of complementary observables. The naive statement that entangled states always have larger correlations than separable states is false, since it is known that entangled states exist (e.g. \(|ψ⟩\) defined above) that are arbitrarily close to separable pure states [2] and to the maximally mixed state (in the sense that for any distance \(ε\) one can choose a sufficiently large dimension \(d\) such that an entangled state is within distance \(ε\) from the maximally mixed state [27]). These have vanishing correlations for most measures of correlation. A notable exception, described above, is the Pearson coefficient that is able to detect the entanglement of \(|ψ⟩\) for all \(ε > 0\) (but it misses many other types of entangled states, such as the Werner states for \(1/3 < p < 1/2\) as shown in Fig. 3).

While our analysis for simplicity focused on correlations of couples of complementary properties, most results can be immediately extended to more than two complementary observables by considering additional MUBs [1]. For example, the results that use Maassen and Uffink’s uncertainty relation can be extended by considering all possible pairwise uncertainty relations.

In summary, we have studied different types of correlations (mutual information \(I\), Pearson coefficient \(C\), and sum of conditional probabilities \(S\)) among complementary observables of two systems. We have shown how they provide information on the entanglement and quantum correlations of a bipartite system. We have derived the following results and presented a few reasonable conjectures: (i) we proved necessary and sufficient conditions for maximal entanglement for \(I, C, S\), (ii) we proved sufficient conditions for entanglement based on \(I\) and conjectured sufficient conditions based on \(C\) and on \(S\); (iii) when gauging complementary correlations using \(I\), we proved that the separable states on the boundary with the entangled-states region are strictly classically correlated, but the same result is false if one uses \(C\) or \(S\); moreover we have shown how \(S\) provides insight on CC, CQ, QC, and QQ states, showing that (iv) without entanglement only classically correlated CC states can have maximal correlation on one variable (but then they have no correlation on the complementary one), whereas (v) separable QQ states can have only partial correlations on complementary variables.

Our method also leads to tests of entanglement that are very easy to implement experimentally: simple measurements of two different observables on the two subsystems are sufficient.

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Appendix. Proofs

Sufficient condition for entanglement using mutual information

Here we prove that if \(I_{AB} + I_{CD} > \log_2 d\), then the state of the two systems is entangled. This theorem can equivalently be stated as: if the state is separable then \(I_{AB} + I_{CD} ≤ \log_2 d\).

From Eq. (1) we have that \(H(A)\) is the entropy of the \(A\) measurement outcomes and \(H(A|B)\) is the conditional
entropy of the $A$ outcomes, which can be also written as

$$H(A|B) = -\sum_{a,b} p(a|b)p(b) \log_2 p(a|b) = \sum_b p(b)H(A|B = b),$$

where

$$H(A|B = b) = -\sum_a p(a|b) \log_2 p(a|b)$$

is the entropy of the probability distribution $p(a|b)$ for fixed $b$. By definition, separable states can be written as $\rho = \sum_i p_i \rho_i \otimes \sigma_i$. The conditional state $\rho^{(b)}$ when the result $b$ is obtained from a $B$ measurement on the second subsystem is

$$\rho^{(b)} = \sum_l \beta_l^{(b)} \rho_l, \quad \beta_l^{(b)} = p_l(b|\sigma_l|b) / \sum_{l'} p_{l'}(b|\sigma_{l'}|b).$$

In the above expression for $\beta_l^{(b)}$ the term in the denominator is $p(b)$, namely the probability of getting outcome $b$ when measuring $B$ on the second subsystem. (Note that, in contrast to entangled states, the components $\rho_l$ of the first subsystem have not changed, only the spectrum has changed.) The concavity of the entropy gives

$$H(A|B = b) = H(A)_{\rho^{(b)}} \geq \sum_l \beta_l^{(b)} H(A)_{\rho_l}$$

$$\Rightarrow H(A|B) = \sum_b p(b)H(A|B = b) \geq \sum_l p_l H(A)_{\rho_l},$$

where $H(X)_{\rho}$ denotes the Shannon entropy of a measurement of $X$ on the state $\rho$. The same reasoning for $C$ and $D$ yields

$$H(C|D) \geq \sum_l p_l H(C)_{\rho_l}.$$ (11)

Now we use Maassen and Uffink’s (MU) entropic uncertainty relation\(^3\) \(^{21}\), which says that for any state $\rho$ we have $H(A)_{\rho} + H(C)_{\rho} \geq -2 \ln c$ with $c = \max_{j,k} |\langle a_j|c_k\rangle|^2$. For complementary observables, $-2 \ln c = \log_2 d$. This means that

$$H(A|B) + H(C|D) \geq \sum_l p_l[H(A)_{\rho_l} + H(C)_{\rho_l}] \geq \log_2 d,$$

where the first inequality is due to the concavity of the entropy, the second is the MU inequality. The above chain of inequalities and the fact that $H(A) \leq \log_2 d$, $H(C) \leq \log_2 d$ imply that

$$I_{AB} + I_{CD} = H(A) - H(A|B) + H(C) - H(C|D) \leq \log_2 d,$$ (12)

which concludes the proof.

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\(^3\) A generalization of the MU relation for more than two observables (e.g. considering mutually unbiased bases) is problematic: there exist mutually unbiased bases where the average entropy is the same as if one considers only two of them, e.g. see \(^5\).
input state $\rho$, namely a state of the form

$$p \sum_{i=0}^{d-1} p_i |a_i\rangle \langle a_i| \otimes \sigma_i + (1-p) \sum_{i=0}^{d-1} p'_i |c_i\rangle \langle c_i| \otimes \sigma'_i \tag{16}$$

(which, by an appropriate choice of $p_i$ and $p'_i$ may also describe states such as $|a_0\rangle |a_0\rangle \otimes \sigma_0 + |c_0\rangle (c_0\rangle \otimes \sigma'_0)/2$).

By taking the partial trace over the second subsystem and then multiplying to the left by $|a_m\rangle$ and to the right by $|c_m\rangle$ for each $m$, one sees that this state cannot have identity as a marginal to saturate inequality (c) unless all terms in the first sum are nonzero. Analogously, using $\langle c_m|\rangle$ and $|c_m\rangle$ one sees that also all terms in the second sum are nonzero. Now, in order to saturate the concavity (a) of Eq. (11), all states $\rho_i$ must have the same entropy for measurement of $A$ as $\rho^{(b)}$ but, to saturate the MU inequality (b), it must also be equal to a pure state (either an eigenstate of $A$ or of $C$). This is impossible for a state of the form (16) unless $p = 0$ or 1, in which case we go back to the case considered above, that leads to the optimal states $\rho_{cc}$ of (13).

**Necessary and sufficient conditions for maximal entanglement**

Here we prove the results on maximal entanglement. We start from the mutual information $I$ and the sum of conditional probabilities $S$. The case of the Pearson coefficient is treated separately below.

Start by proving that if $I_{AB} + I_{CD} = 2 \log_2 d$ or $S_{AB} + S_{CD} = 2d$ then the state is maximally entangled (the converse will be proven below). From the definition of $I_{AB}$ in Eq. (1), it is upper bounded by $\log_2 d$ and can achieve this bound only when the conditional entropy is null. Since the conditional entropy is defined as

$$H(A|B) = -\sum_{a,b} p(a,b) \log_2 p(a|b) \tag{17}$$

it is null only when the conditional probabilities are 0 or 1 which implies the result for $S_{AB} + S_{CD}$. We first prove this for two qubits for simplicity, with the two complementary properties identified by projectors on the computational basis $\{|0\rangle, |1\rangle\}$ and on the Fourier basis $\{|\pm\rangle = |0\rangle \pm |1\rangle\}$. We prove that if $p(0|0) = p(1|1) = p(+|+) = p(-|-) = 1$, the state of the two systems is a maximally entangled state $|\Psi^+\rangle$. The conditional probability is $p(0|0) = \text{Tr}[|0\rangle \langle 0| \rho_0]$, where $\rho_0$ is the state conditioned on obtaining 0 on the second system:

$$\rho_0 = \frac{p(0|0) |0\rangle \langle 0|_B \text{Tr}[|B\rangle \langle B|_B]}{p(0|0) = \frac{\langle 00|\rho_0 \rangle \langle 00| \rho_0 + \langle 10|\rho_1 \rangle \langle 10| \rho_1}} \tag{18}$$

where $\rho$ is the initial state of the composite system. From the above expression we have that $p(0|0) = 1$ only if $\langle 10|\rho_1 \rangle = 0$. By the same argument for $p(1|1)$ we can conclude that $\langle 01|\rho_01 \rangle = 0$, so that $\rho$ must belong to the subspace spanned by $\{|00\rangle, |11\rangle\}$. Note that $\langle 10|\rho_1 \rangle = \langle 01|\rho_01 \rangle = 0$ implies that also $\langle 10|\rho_01 \rangle + \langle 10|\rho_10 \rangle = 0$ (see below). This means that

$$\langle +|\rho|+\rangle = \langle 00|\rho_00 \rangle + \langle 11|\rho|11 \rangle + \langle 00|\rho|11 \rangle + \langle 11|\rho|00 \rangle$$

$$\langle -|\rho|-\rangle = \langle 00|\rho_00 \rangle - \langle 11|\rho|11 \rangle - \langle 00|\rho|11 \rangle - \langle 11|\rho|00 \rangle$$

which is $p(+|+) = 1$ if and only if $\langle 00|\rho_00 \rangle + \langle 11|\rho|11 \rangle = \langle 00|\rho|11 \rangle + \langle 11|\rho|00 \rangle$. The above relation holds if and only if $\rho$ is a pure state, and is equal to $\rho = |\Psi^+\rangle \langle \Psi^+|$. In order to prove that we employ the inequality $\rho_{nn} + \rho_{mm} \geq \rho_{nm} + \rho_{mn}$, which is an inequality only for states that are pure and balanced when restricted to the $\{|m\rangle, |n\rangle\}$ subspace, namely for states that in such subspace are $|m\rangle + |n\rangle$. This inequality can be easily proved by decomposing $p = \sum_i \lambda_i |i\rangle \langle i|$ and using the same inequality for pure states: $|\alpha|^2 + |\beta|^2 \geq \alpha^* \beta + \beta^* \alpha$ (where $\alpha = \langle n|\psi\rangle$, $\beta = \langle m|\psi\rangle$), which can be easily derived noticing that $0 \leq |\alpha - \beta|^2 = |\alpha|^2 + |\beta|^2 - \alpha^* \beta - \beta^* \alpha$, where equality holds if and only if $\alpha = \beta$.

We will now extend the above proof to couples of systems in arbitrary finite dimension $d$. The matrix elements of the global state $\rho$ in the computational basis are denoted for brevity as $\langle ij|\rho|kl\rangle = \rho_{ij,kl}$. The conditions that the conditional probabilities in the computational basis must be one are given by

$$p(0|0) = \frac{\rho_{00,00}}{\sum_{i=0}^{d-1} \rho_{i0,i0}} = 1 \tag{19}$$

The above condition is satisfied iff $\sum_{i=1}^{d-1} \rho_{i0,i0} = 0$, which implies that $\rho_{i0,i0} = 0$ for $i \neq 0$. The same argument holds for the conditional probability $p(j|j)$ and we then have

$$p(j|j) = \frac{\rho_{jj,jj}}{\sum_{j=0}^{d-1} \rho_{jj,jj}} = 1 \tag{20}$$

The above condition is satisfied iff $\sum_{j=0}^{d-1} \rho_{ij,ij} = 0$ for fixed $j$, which implies that $\rho_{ij,j} = 0$ for $i \neq j$. As a consequence, the positivity of $\rho$ requires that $\rho_{ij,kl} = 0$ for $i \neq j, k \neq l$. The above conditions then imply that the only nonvanishing elements of $\rho$ are of the form $\rho_{ii,jj}$.

Let us now denote as $\{|j\rangle, j = 0, d-1\}$ the Fourier transform of the computational basis, namely

$$|j\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} e^{i 2\pi k j/d} |k\rangle \tag{21}$$

The matrix elements in the Fourier transformed basis can
be written as
\[ \rho_{\bar{b}\bar{b}} = \frac{1}{d^2} \sum_{j,k=0}^{d-1} \rho_{jj, kk} \]
\[ \rho_{\bar{j}\bar{j}} = \frac{1}{d^2} \sum_{j,k=0}^{d-1} e^{i2\pi(k-j)i/d} \rho_{jj, kk} . \]

The conditional probability \( p(\bar{0}|\bar{0}) \) then takes the form
\[ p(\bar{0}|\bar{0}) = \frac{\sum_{j,k=0}^{d-1} \rho_{jj, kk}}{\sum_{i=0}^{d-1} \sum_{j,k=0}^{d-1} e^{i2\pi(k-j)i/d} \rho_{jj, kk}} . \]

By using the identity
\[ \sum_{i=0}^{d-1} e^{i2\pi li/d} = d\delta_{l, kd} , \]
which means that the l.h.s. of Eq. (23) vanishes for all values of \( l \) that are not multiples of the dimension \( d \), we can write the denominator in Eq. (23) as
\[ \sum_{j,k=0}^{d-1} \rho_{jj, kk} \sum_{i=0}^{d-1} e^{i2\pi(k-j)i/d} = \sum_{j=0}^{d-1} \rho_{jj, jj} , \]

By imposing that the probability in Eq. (23) must be one we have that
\[ p(\bar{0}|\bar{0}) = \frac{\sum_{j,k=0}^{d-1} \rho_{jj, kk}}{\sum_{j=0}^{d-1} \rho_{jj, jj}} = 1 . \]

By the same reasoning as for the qubit case the above condition implies that \( \rho \) is a projector onto the maximally entangled state \( |\Phi^+\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |jj\rangle \).

To finish the proof for \( I \) and \( S \), we have to prove the converses: if the state is maximally entangled, then there exist two complementary bases such that \( I_{AB} + I_{CD} = 2 \log_2 d \) or \( S_{AB} + S_{CD} = 2d \). Any maximally entangled state \( |\Psi\rangle \) is local-unitarily equivalent to \( |\Phi^+\rangle \equiv \sum_{j} |jj\rangle/\sqrt{d} \). Namely, \( |\Psi\rangle = U \otimes U' |\Phi^+\rangle \) with \( U \) and \( U' \) unitaries (which transform local bases one into another). The same result as for \( |\Phi^+\rangle \) can then be achieved by starting from \( |\psi\rangle \) and considering as complementary bases the ones that are obtained by applying \( U \otimes U' \) to the computational and the Fourier bases.

Finally, to prove the necessary and sufficient condition for the Pearson coefficient \( \rho \), we note that we have just shown that a state has maximal correlation for two complementary bases if and only if it is local-unitarily equivalent to \( |\Phi^+\rangle \). Namely, in two complementary bases, the local outcomes match: \( S_{AB} + S_{CD} = 2d \). It is known that the Pearson coefficient takes its extremal values \( \pm 1 \) iff the two stochastic variables are linearly dependent and perfectly correlated (i.e. in one-to-one correspondence).

**Sum of conditional probabilities for CC and CQ states**

Here we prove that CC states can have maximal correlations only on one of two complementary variables and that CQ states cannot have maximal correlations on any variable. The first statement is formalized above as: \( p(a_i|b_i) = 1 \forall i \) then we must have \( p(c_i|d_i) = 1/d \forall i \), where \( a_i, b_i, c_i, d_i \) are the results of the measurements of \( A, B, C, D \). The second statement is formalized as: even if \( p(c_i|d_i) = 1/d \forall i \) we still cannot obtain \( p(a_i|b_i) = 1 \forall i \).

We can prove both statements at the same time by observing that CC and CQ states can be written in the form
\[ \rho_d = \sum_a p_a|a\rangle \langle a| \otimes \rho_a , \]
which can have maximal correlation on some property only for CC states (where the \( \rho_a \) are orthogonal for different \( a \)). We can then show that the state \( \rho_d \) which has some correlation on \( a \) cannot have any correlation on \( c \) when \( c \) is a complementary property, namely if \( |\langle c|a\rangle|^2 = 1/d \). Actually,
\[ \rho_d = \sum_a \sum_{c'c'} p_a/d |c\rangle \langle c'| e^{i\theta(a,c)-\theta(a,c')} \otimes \rho_a \]
\[ = \sum_a \sum_{c'c'} 1/d |c\rangle \langle c'| \otimes (\sum_a p_a \rho_a + \sum_a \sum_{c\neq c'} \cdots) , \]
where \( \theta \) is some phase factor and where, as above, in the second line we have separated the part diagonal in \( c \) (which is the only one that contributes to the correlations for \( c \)) from the rest. It is clear from the form of the state in (28) that such a state does not have any correlations in \( c \): namely that a measurement of \( C \) on the first system gives no information on the second.

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1. T. Durt, B.-G. Englert, I. Bengtsson, K. Życzkowski, On mutually unbiased bases, Int. J. Quantum Information 8, 535 (2010).
2. D. Bruss, Characterizing entanglement, J. Math. Phys. 43, 4237 (2002); R. Horodecki, P. Horodecki, M. Horodecki, K. Horodecki, Quantum entanglement, Rev. Mod. Phys. 81, 865 (2009).
3. K. Modi, A. Brodutch, H. Cable, T. Paterek, V. Vedral, Rev. Mod. Phys. 84, 1655 (2012).
4. A. Peres, Phys. Rev. Lett. 77, 1413 (1996); M. Horodecki, P. Horodecki, R. Horodecki, Phys. Lett. A 223, 1 (1996).
5. G. Vidal, R.F. Werner, Computable measure of entanglement, Phys. Rev. A 65, 032314 (2002).
6. H.F. Hofmann, S. Takeuchi, Violation of local uncertainty relations as a signature of entanglement, Phys. Rev. A 68, 032103 (2003).
7. J. Schlienz and G. Mahler, Description of entanglement, Phys. Rev. A 52, 4396 (1995).
[8] C. Kothe, G. Björk, Entanglement quantification through local observable correlations, Phys. Rev. A 75, 012336 (2007); I.S. Abascal, G. Björk, Bipartite entanglement measure based on covariance Phys. Rev. A 75, 062317 (2007).
[9] J.I. de Vicente, Separability criteria based on the Bloch representation of density matrices, Quantum Inf. Comput. 7, 624 (2007); J.I. de Vicente, M. Huber, Multiparticle entanglement detection from correlation tensors, Phys. Rev. A 84, 062306 (2011).
[10] V. Giovannetti, Phys. Rev. A 70, 012102 (2004).
[11] B.M. Terhal, Linear Algebra Appl. 323, 61 (2000), arXiv:quant-ph/9810091; O. Gühne, G. Tóth, Physics Reports 474, 1 (2009).
[12] M. Lewenstein, B. Kraus, J.I. Cirac, P. Horodecki, Optimization of entanglement witnesses, Phys. Rev. A 62, 052310 (2000).
[13] W.K. Wootters, Entanglement of Formation of an Arbitrary State of Two Qubits, Phys. Rev. Lett. 80, 2245 (1998).
[14] O. Rudolph, Quantum Inf. Process. 4 219 (2005), arXiv:quant-ph/0202121.
[15] O. Gühne, Phys. Rev. Lett. 92, 117903 (2004).
[16] O. Gühne, P. Hyllus, O. Gittsovich, J. Eisert, Covariance Matrices and the Separability Problem, Phys. Rev. Lett. 99, 130504 (2007).
[17] O. Gittsovich, O. Gühne, P. Hyllus, J. Eisert, Unifying several separability conditions using the covariance matrix criterion, Phys. Rev. A 78, 052319 (2008).
[18] W.H. Zurek, Ann. Phys. 9, 855 (2000).
[19] S. Wu, Z. Ma, Z. Chen, S. Yu, Sci. Rep. 4, 4036 (2014).
[20] C. Spengler, M. Huber, S. Brierley, T. Adaktylos, B.C. Hiesmayr, Entanglement detection via mutually unbiased bases Phys. Rev. A 86, 022311 (2012); B.C. Hiesmayr, W. Löffler, New J. Phys. 15, 083036 (2013).
[21] H. Maassen, J.B.M. Uffink, Phys. Rev. Lett. 60, 1103 (1988).
[22] E. Schrödinger, "Zum Heisenbergschen Unschärfeprinzip", Sitzungsberichte der Preussischen Akademie der Wissenschaften, Physikalisch-Mathematische Klasse 14: 296, 303 (1930).
[23] K. Życzkowski, P. Horodecki, A. Sanpera, M. Lewenstein, Volume of the set of separable states, Phys. Rev. A 58, 883 (1998).
[24] D.V. Foster, P. Grassberger, Phys. Rev. E 83, 010101(R) (2011).
[25] B. Dakić, V. Vedral, C. Brukner, Phys. Rev. Lett. 105, 190502 (2010).
[26] M.A. Nielsen, J. Kempe, Separable States Are More Disordered Globally than Locally, Phys. Rev. Lett. 86, 5184 (2001).
[27] A.O. Pittenger, M.H. Rubin, Phys. Rev. A 62, 032313 (2000).
[28] C. Lupo, S. Lloyd, arXiv:1312.4431 (2013).
[29] A.R. Gonzales, J.A. Vaccaro and S.M. Barnett, Phys. Lett. A 205, 247 (1995).