Complementarity and Correlations

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We provide an interpretation of entanglement based on classical correlations between measurement outcomes of complementary properties: States that have correlations beyond a certain threshold are entangled. The reverse is not true, however. We also show that, surprisingly, all separable nonclassical states exhibit smaller correlations for complementary observables than some strictly classical states. We use mutual information as a measure of classical correlations, but we conjecture that the first result holds also for other measures (e.g., the Pearson correlation coefficient or the sum of conditional probabilities).

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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 $|c_i\rangle$ 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 [1]. Here we study what classical correlations in the measurements of these complementary properties tell us about the quantum correlations of the state of the system.

Typically one discusses entanglement [2] in terms of nonlocality, Bell inequality violations, monotones over local operations and classical communication, etc. For example, previous literature on entanglement focused on time reversal (for the positive partial transpose criterion [3,4]), local uncertainty relations [5–9], entropic uncertainty relations [10–13], entanglement witnesses [14–17], concurrence [18], the cross-norm criterion [19], and the covariance matrix criterion [20–24] (the latter encompassing many of the former). In contrast to these studies, we focus specifically on classical correlations for complementary properties. Classical correlations are typically quantified in terms of the mutual information, which is the main quantity considered here. We will also discuss the case of alternative measures such as the Pearson correlations and the sum of conditional probabilities. In [25] related approaches using specific measures of correlations (different from the ones used here) were proposed.

The outline of the Letter 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 quantum correlations. We provide some examples of applications. The details of the proofs of our results are reported in the Supplemental Material [33].

Complementary correlations.—Consider two systems of finite dimension d [44] and two observables $A \otimes B$ and $C \otimes D$ (Fig. 1) where A and C are complementary on the first system (namely, $|\langle a_i|c_j\rangle| = 1/\sqrt{d}$ 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 the 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, which we name 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, $(|\mathcal{X}_{AB}|^{1/2} - |\mathcal{X}_{CD}|^{1/2})^2 \geq 0$ implies $2\sqrt{|\mathcal{X}_{AB}\mathcal{X}_{CD}|} \leq |\mathcal{X}_{AB}| + |\mathcal{X}_{CD}|$. Thus, we will mainly consider the sum of the correlations for complementary observables $|\mathcal{X}_{AB}| + |\mathcal{X}_{CD}|$ as a way to evaluate the complementary correlations.

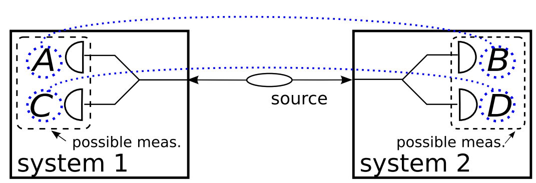

FIG. 1 (color online). Complementary correlation measurements. Each of two systems is subject to the measurement of one of two observables: either A or C on system 1 and either B or D on system 2. Correlations are evaluated between the results of A and B and between C and D (dashed lines). A and C are complementary on the first system, B and D on the second.

Mutual information.—We start considering the mutual information: $I_{AB} \equiv H(A) - H(A|B)$, 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

$$I_{AB} + I_{CD} > \log_2 d, \tag{1}$$

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

$$\rho_{cc} = \sum_i |a_i\rangle\langle a_i| \otimes |b_i\rangle\langle b_i|/d, \tag{2}$$

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. 2(a), 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 Supplemental Material [33]) 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 [26] (see Supplemental Material for the details [33]). 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 and no discord. This means that quantum correlated states without entanglement do not have higher correlations for 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 quantum-quantum (QQ) states sits on the border, as shown in Fig. 2(b)]. It can be proved by analyzing the conditions for the equality of the concavity of the entropy and of Maassen and Uffink's inequality (see Supplemental Material [33]).

Pearson correlation.— The second measure of correlation we consider is the Pearson correlation coefficient $\mathcal{C}_{AB}$, defined as

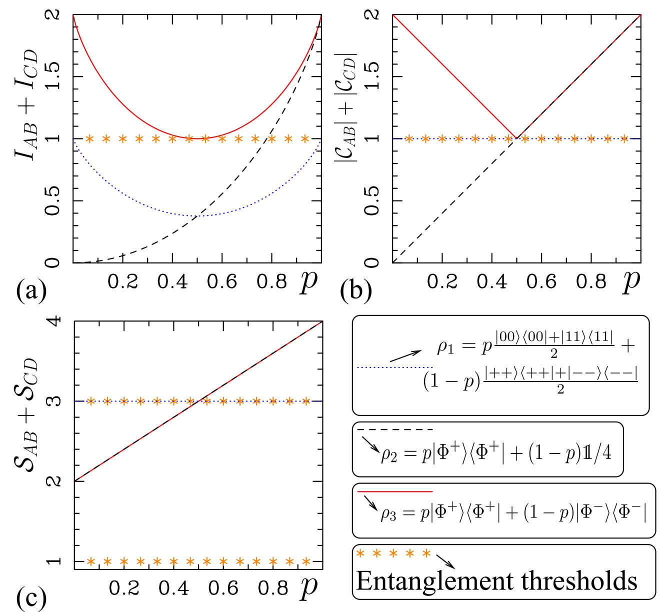

FIG. 2 (color online). Examples of complementary correlations for different measures of correlation and different families of states. (a) Correlation $I_{AB} + I_{CD}$ plotted as a function of the parameter p for the families of p-dependent two-qubit states indicated in the lower right panel. The dotted-line states are always separable and are nonzero discord QQ states for $p \neq 0, 1$; the dashed-line states (Werner states) are entangled for $p > 1/3$, whereas the solid-line states are entangled for $p \neq 1/2$. Above the threshold 1 (stars), the states are certainly entangled. (b) Same as previous for $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}|$, note that the QQ state (dotted line) is on the conjectured threshold 1 (stars) for this measure of correlation. (c) Same as previous for $\mathcal{S}_{AB} + \mathcal{S}_{CD}$. Here there are two entanglement boundaries: The states that have a sum larger than 3 or smaller than 1 are conjectured to be entangled. Again, the dotted state coincides with one of the conjectured boundaries. The dashed line and the solid line are superimposed. Here $|\pm\rangle \equiv (|0\rangle \pm |1\rangle)/\sqrt{2}$ and $|\Phi^\pm\rangle \equiv (|00\rangle \pm |11\rangle)/\sqrt{2}$.

$$\mathcal{C}_{AB} \equiv \frac{\langle AB\rangle - \langle A\rangle\langle B\rangle}{\sigma_A \sigma_B}, \tag{3}$$

where, as before, A and B denote observables relative to the two systems, $\langle X\rangle = \mathrm{Tr}[X\rho]$ is the expectation value on the quantum state ρ, and σ_X^2 is the variance of the observable X. The above quantity cannot be applied to eigenstates of A or B. Clearly, $\mathcal{C}_{AB} = 0$ for uncorrelated (product) states. 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:

$$\begin{aligned} |\langle AB\rangle - \langle A\rangle\langle B\rangle|^2 &= \left|\frac{\langle [A,B]\rangle + \langle\{A,B\}\rangle}{2} - \langle A\rangle\langle B\rangle\right|^2 \\ &= \left|\frac{1}{2}\langle [A,B]\rangle\right|^2 + \left|\frac{1}{2}\langle\{A,B\}\rangle \right. \\ &\quad \left. - \langle A\rangle\langle B\rangle\right|^2 \le \sigma_A^2\sigma_B^2, \end{aligned} \tag{4}$$

where $[\cdot,\cdot]$ and $\{\cdot,\cdot\}$ denote the commutator and anticommutator, respectively, and where the final inequality is the Schrödinger uncertainty relation [27].

We now use $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}|$ 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 $A = \sum_j j|a_j\rangle\langle a_j|$ and $B = A^3$). 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 $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| = 2$, e.g., if one uses $A = B = \sum_j j|a_j\rangle\langle a_j|$, $C = D = \sum_j j|c_j\rangle\langle c_j|$ where $|a_j\rangle$ and $|c_j\rangle$ are 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 ± 1 if and only if there is a functional relation that connects the two stochastic variables (details in Supplemental Material [33]).

Instead, for nonmaximally entangled states we have two conjectures which are supported by numerical evidence: (i) If $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| > 1$, the two systems are entangled. As for the mutual information, the inequality is tight since ρ_{cc} is separable and has $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| = 1$. (ii) If $|\mathcal{C}_{AB}\mathcal{C}_{CD}| > 1/4$, the two systems are entangled. Also this inequality is tight: It is attained by the separable state $\sum_i (|a_i a_i\rangle\langle a_i a_i| + |c_i c_i\rangle\langle c_i c_i|)/2d$, 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 $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| \le 1$ implies $|\mathcal{C}_{AB}\mathcal{C}_{CD}| \le 1/4$.

The proof of these conjectures is complicated by the fact that the convexity properties of $\mathcal{C}_{AB}$ are unknown. Nonetheless, they are natural conjectures that are easy to verify for large classes of states [e.g., see Fig. 2(b)]. We have also performed extensive numerical checks by testing them on large sets of random states generated according to the prescription described in [28], and verifying that no state with nonpositive partial transpose [3] lies over the conjectured threshold.

Note that 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 [29]. Indeed, consider the family of entangled two-qubit states

$$|\psi_\epsilon\rangle = \epsilon|00\rangle + \sqrt{1-\epsilon^2}|11\rangle, \tag{5}$$

with $\epsilon \in [0,1]$. If one uses $A = B = |1\rangle\langle 1|$ and $C = D = |+\rangle\langle +|$, for all $0 < \epsilon < 1$ such state has $|\mathcal{C}_{AB}| + |\mathcal{C}_{CD}| = 1 + 2\epsilon\sqrt{1-\epsilon^2} > 1$ [45], 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 $0 < \epsilon < 1$ (assuming the above conjectures), whereas the mutual information does not even identify it as classically correlated *at all* for $\epsilon \to 0$. Indeed, numerical simulations suggest that the 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 $\mathcal{S}_{AB}$, defined as

$$\mathcal{S}_{AB} \equiv \sum_i p(a_i|b_i), \tag{6}$$

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 [17] a similar approach was used, but employing joint probabilities in place of conditional ones.

Gauging complementary correlations with the sum $\mathcal{S}_{AB} + \mathcal{S}_{CD}$ we can again obtain information about entanglement and quantum correlations: (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 $\mathcal{S}_{AB} + \mathcal{S}_{CD} = 2d$. (ii) As for the Pearson correlation, we have a conjecture for nonmaximally entangled states: If $\mathcal{S}_{AB} + \mathcal{S}_{CD}$ 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 ρ_{cc} and the lower bound by the separable state $\sum_i |a_i b_{i\oplus 1}\rangle\langle a_i b_{i\oplus 1}|/d$, with $\oplus$ sum modulo d.

Let us analyze the case of separable states. We remind the reader that classical-quantum (CQ) and quantum-classical (QC) states have the forms $\sum_i p_i |a_i\rangle\langle a_i| \otimes \rho_i$ and $\sum_i p_i \rho_i \otimes |a_i\rangle\langle a_i|$, respectively, where $\{|a_i\rangle\}$ is a set of orthogonal states for one subsystem and $\{\rho_i\}$ is not an orthogonal set of states. Note that separable 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 $p(c_i|d_i) = 1/d\ \forall\, i$, 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 $p(a_i|b_i) = 1\ \forall\, i$, even when $p(c_i|d_i) = 1/d$], and (v) QQ states can have only *partial* correlation for each complementary property. For example, the separable two-qubit state $(|00\rangle\langle 00| + |11\rangle\langle 11| + |++\rangle\langle ++| + |--\rangle\langle --|)/4$ has a partial correlation on both complementary variables, since $p(0|0) = p(1|1) = p(+|+) = p(-|-) = 3/4$.

Given the properties (iii) and (iv), one might suspect that separable states with nonvanishing quantum correlations have always less complementary correlations, 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 Supplemental Material [33]) as for the cases seen previously. The difficulty in proving the conjecture (ii) stems again from a lack of definite concavity properties of $\mathcal{S}_{AB}$, 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 $1/d \le p(a_i|b_i) + p(c_i|d_i) \le 1 + 1/d$ 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 $(|00\rangle\langle 00| + |++\rangle\langle ++|)/2$ of two qubits for which $p(0|0) + p(+|+) = 5/3$. If one uses joint probabilities in place of conditional ones, a sufficient condition for entanglement can indeed be proven [17]. 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 Supplemental Material [33]), whereas property (v) is a direct consequence of the example provided above.

Extension to more complementary observables.—Up to now we have considered the correlations of the measurement outcomes of two complementary observables. All systems have at least three complementary observables [1], and it is known that there are $d + 1$ for d-dimensional systems if d is a power of a prime [1,30]. Our results can be immediately extended to an arbitrary number of complementary observables by calculating the correlations of all the known complementary observables and considering the sum of the two largest ones. For example, for mutual information, we can extend the condition, Eq. (1), to conclude that the state is entangled if

$$\max(I_{AB}, I_{CD}, I_{EF}, \ldots) + \max_2(I_{AB}, I_{CD}, I_{EF}, \ldots) > \log_2 d, \tag{7}$$

where $\max_2$ denotes the second largest term and where $A \otimes B$, $C \otimes D$, $E \otimes F$, etc. are all observables complementary to each other. The extensions of all other results and conjectures are analogous.

Moreover, at least in the case of qubits the bound at point (ii) for the mutual information and the conjectured bound at point (i) for the Pearson correlations can be made stronger by adding correlations for the third complementary observable. This can improve significantly the efficiency of the present method if used for entanglement detection. For details and for a comparison with other known entanglement detection schemes based on measurements of mutually unbiased bases, see the Supplemental Material [33].

Conclusions.—In summary, we have introduced an interpretation of entanglement based on classical correlations of the measurement outcomes of complementary observables. We have studied different types of correlations (mutual information I, Pearson coefficient $\mathcal{C}$, and the sum of conditional probabilities $\mathcal{S}$) for 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, $\mathcal{C}$, $\mathcal{S}$, (ii) we proved sufficient conditions for entanglement based on I and conjectured sufficient conditions based on $\mathcal{C}$ and on $\mathcal{S}$, (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 $\mathcal{C}$ or $\mathcal{S}$; moreover, we have shown how $\mathcal{S}$ provides insight on CC, CQ, QC, and QQ states, showing that (iv) without entanglement only classically correlated states CC 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.

One can ask if it is possible to give necessary and sufficient conditions based on correlations for 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., $|\psi_\epsilon\rangle$ defined above) that are arbitrarily close to separable pure states [31] 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 [32]). 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 $|\psi_\epsilon\rangle$ for all $\epsilon > 0$ (but it misses other types of entangled states).

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