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Strengthened Bell inequalities for orthogonal spin directions

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Abstract

We provide bounds on correlations of locally orthogonal observables in two-qubit separable states. These bounds strengthen the Bell inequality and improve upon some alternative entanglement criteria. They provide necessary and sufficient criteria for separability of pure states and test the correlations allowed by local hidden variable models against those allowed by separable quantum states.

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1. Introduction

The current interest in the study of entangled quantum states derives from two sources: their role in the foundations of quantum mechanics [1] and their applicability in practical problems of information processing (such as quantum communication and computation) [2].

Bell inequalities likewise serve a dual purpose. Originally, they were designed in order to answer a foundational question: to test the predictions of quantum mechanics against those of a local hidden-variable (LHV) theory [3]. However, these inequalities also provide a test to distinguish entangled from separable quantum states [4,5]. Indeed, experimenters routinely use violations of a Bell inequality to check whether they have succeeded in producing entangled states. This problem of entanglement detection is crucial in all experimental applications of quantum information processing.

It is the goal of this Letter to report that in the case of the standard Bell inequality experiment, i.e., for two distant spin-$1/2$ particles, significantly stronger inequalities hold for separable states in the case of locally orthogonal observables. These inequalities provide sharper tools for entanglement detection, and are readily applicable to recent experiments such as [6]. In fact, if they hold for all sets of locally orthogonal observables they are necessary and sufficient for separability, so the violation of these separability inequalities is not only a sufficient but also a necessary condition for entanglement. They furthermore advance upon the necessary and sufficient separability inequalities of Yu et al. [7], since, in contrast to these, the inequalities presented here do not need to assume that the orientations of the measurement basis for each qubit are the same, so no shared reference frame is necessary.

We show the strength and efficiency of the separability criteria by showing that they are stronger than other sufficient and experimentally accessible criteria for two-qubit entanglement while using the same measurement settings. These are (i) the so-called fidelity criterion [8], and (ii) recent linear and nonlinear entanglement witnesses [9–11]. However, in order to implement all of the above criteria successfully, the observables have to be chosen in a specific way which depends on the state to be detected. So in general one needs some prior knowledge about this state. In order to circumvent this experimental drawback we discuss the problem of whether a finite subset of the separability inequalities could already provide a necessary and sufficient condition for separability. For mixed state we have not

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been able to resolve this, but for pure states a set of six inequalities using only three sets of orthogonal observables is shown to be already necessary and sufficient for separability.

The inequalities, however, are not applicable to the original purpose of testing LHV theories. This shows that the purpose of testing entanglement within quantum theory, and the purpose of testing quantum mechanics against LHV theories are not equivalent, a point already demonstrated by Werner [12]. Our analysis follows up on Werner's observation by showing that the correlations achievable by all separable quantum states in a standard Bell experiment are tied to a bound strictly less than those achievable for LHV models. In other words, quantum theory needs entangled states even to produce the latter type of correlations. As an illustration, we exhibit a class of entangled states, including the Werner states, whose correlations in the standard Bell experiment possess a reconstruction in terms of a local hidden-variable model.

This Letter is organized as follows. In Section 2, we rehearse the Bell inequalities for separable states in the standard setting and derive a stronger bound for orthogonal observables. In Section 3, we compare this result with that of LHV theories and argue that the stronger bound does not hold in that case. In Section 4, we return to quantum theory and derive an even stronger bound than in Section 2 which provides a necessary and sufficient criterion for separability of all quantum states, pure or mixed. Furthermore, it is shown that the orientation of the measurement basis is not relevant for the criterion to be valid. Section 5 compares the strength of these inequalities with some other criteria for separability, not based on the Bell inequalities. Also, it is investigated whether a finite subset of the inequalities of Section 4 could already provide a necessary and sufficient separability condition. Section 6 summarizes our conclusions.

2. Bell inequalities as a test for entanglement

Consider a system composed of a pair of spin-1/2 particles (qubits) on the Hilbert space $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ in the familiar setting of a standard Bell experiment consisting of two distant sites, each receiving one of the two particles, and where, at each site, a choice of measuring either of two spin observables is made. Let A, A' denote the two spin observables on the first particle, and B, B' on the second. We write AB, etc., as shorthand for $A \otimes B$ and $\langle AB\rangle_\rho := \mathrm{Tr}[\rho A \otimes B]$ or $\langle AB\rangle_\Psi = \langle\Psi|A \otimes B|\Psi\rangle$ for the expectations of AB in the mixed state ρ or pure state $|\Psi\rangle$.

It is well known that for all such observables and all separable states, i.e., states of the form $\rho = \rho_1 \otimes \rho_2$ or convex mixtures of such states, the Bell inequality in the form derived by Clauser, Horne, Shimony and Holt (CHSH) [13] holds:

$$\big|\langle AB + AB' + A'B - A'B'\rangle_\rho\big| \leqslant 2. \tag{1}$$

The maximal violation of (1) follows from an inequality of Cirel'son [14] (cf. Landau [15]) that holds for all quantum states:

$$\big|\langle AB + AB' + A'B - A'B'\rangle_\rho\big| \leqslant 2\sqrt{2}. \tag{2}$$

Equality in (2)—and thus the maximal violation of inequality (1) allowed in quantum mechanics—is attained by, e.g., the pure entangled states $|\phi^\pm\rangle = \frac{1}{\sqrt{2}}(|{\uparrow\uparrow}\rangle \pm |{\downarrow\downarrow}\rangle)$ and $|\psi^\pm\rangle = \frac{1}{\sqrt{2}}(|{\uparrow\downarrow}\rangle \pm |{\downarrow\uparrow}\rangle)$.

In Ref. [16] it was furthermore shown that for all such observables and for all states ρ

$$\langle AB' + A'B\rangle_\rho^2 + \langle AB - A'B'\rangle_\rho^2 \leqslant 4, \tag{3}$$

which strengthens the Cirel'son inequality (2). This quadratic inequality (3) is likewise saturated for maximally entangled states like $|\psi^\pm\rangle$ and $|\phi^\pm\rangle$. Unfortunately, no smaller bound on the left-hand side of (3) exists for separable states, as long as the choice of observables is kept general. (To verify this, take $|\Psi\rangle = |{\uparrow\uparrow}\rangle$ and $A = A' = B = B' = \sigma_z$.) Thus, the quadratic inequality (3) does not distinguish entangled and separable states. We now show that a much more stringent bound can be found on the left-hand side of (3) for separable states when a suitable choice of observables is made, exploiting an idea made in a different context by [17].

For the case of the singlet state $|\psi^-\rangle$, it has long been known that an optimal choice of the spin observables for the purpose of finding violations of the Bell inequality requires that A, A' and B, B' are pairwise orthogonal, and many experiments have chosen this setting. And for general states, it is only in such locally orthogonal configurations that one can hope to attain equality in inequality (2) [18–20]. It is not true, however, that for any given state ρ the maximum of the left-hand side of the Bell–CHSH inequality always requires orthogonal settings [4,5,21].

However this may be, we will from now on assume local orthogonality, i.e., $A \perp A'$ and $B \perp B'$ (for the case of two qubits this amount to the local observables anti-commuting with each other: $\{A, A'\} = 0 = \{B, B'\}$). Furthermore, assume for the moment that the two-particle state is pure and separable. We may thus write $\rho = |\Psi\rangle\langle\Psi|$, where $|\Psi\rangle = |\psi\rangle|\phi\rangle$, to obtain:

$$\begin{aligned}
&\langle AB' + A'B\rangle_\Psi^2 + \langle AB - A'B'\rangle_\Psi^2 \\
&\quad = \big(\langle A\rangle_\psi\langle B'\rangle_\phi + \langle A'\rangle_\psi\langle B\rangle_\phi\big)^2 + \big(\langle A\rangle_\psi\langle B\rangle_\phi - \langle A'\rangle_\psi\langle B'\rangle_\phi\big)^2 \\
&\quad = \big(\langle A\rangle_\psi^2 + \langle A'\rangle_\psi^2\big)\big(\langle B\rangle_\phi^2 + \langle B'\rangle_\phi^2\big).
\end{aligned} \tag{4}$$

Now, for any pure spin-$\frac{1}{2}$ state $|\psi\rangle$ on $\mathcal{H} = \mathbb{C}^2$, and any orthogonal triple of spin components A, A' and A'', one has $\langle A\rangle_\psi^2 + \langle A'\rangle_\psi^2 + \langle A''\rangle_\psi^2 = 1$, and similarly $\langle B\rangle_\phi^2 + \langle B'\rangle_\phi^2 + \langle B''\rangle_\phi^2 = 1$. Therefore, we can write (4) as:

$$\begin{aligned}
&\langle AB' + A'B\rangle_\Psi^2 + \langle AB - A'B'\rangle_\Psi^2 \\
&\quad = \big(1 - \langle A''\rangle_\psi^2\big)\big(1 - \langle B''\rangle_\phi^2\big).
\end{aligned} \tag{5}$$

This result for pure separable states can be extended to any mixed separable state by noting that the density operator of any such state is a convex combination of the density operators for pure product-states, i.e., $\rho = \sum_i p_i|\Psi_i\rangle\langle\Psi_i|$, with $|\Psi_i\rangle = |\psi_i\rangle|\phi_i\rangle$, $p_i \geqslant 0$ and $\sum_i p_i = 1$. We may thus write for such states:

$$
\begin{aligned}
&\langle AB' + A'B\rangle_\rho^2 + \langle AB - A'B'\rangle_\rho^2 \\
&\quad \leqslant \left(\sum_i p_i \sqrt{\langle AB' + A'B\rangle_i^2 + \langle AB - A'B'\rangle_i^2}\right)^2 \\
&\quad = \left(\sum_i p_i \sqrt{\left(1 - \langle A''\rangle_i^2\right)\left(1 - \langle B''\rangle_i^2\right)}\right)^2 \\
&\quad \leqslant \left(1 - \langle A''\rangle_\rho^2\right)\left(1 - \langle B''\rangle_\rho^2\right).
\end{aligned} \tag{6}
$$

Here, $\langle\cdot\rangle_i$ denotes an expectation value with respect to $|\Psi_i\rangle$ (e.g., $\langle A''\rangle_i := \langle\Psi_i|A'' \otimes \mathbb{1}|\Psi_i\rangle$) and $\langle A''\rangle_\rho := \langle A'' \otimes \mathbb{1}\rangle_\rho$. The first inequality follows because $\sqrt{\langle AB' + A'B\rangle_\rho^2 + \langle AB - A'B'\rangle_\rho^2}$ is a convex function of ρ and the second because $\sqrt{(1 - \langle A''\rangle_\rho^2)(1 - \langle B''\rangle_\rho^2)}$ is concave in ρ. (To verify this, it is helpful to use the general lemma that for all positive concave functions f and g, the function $\sqrt{fg}$ is concave.)

Thus, we obtain for all separable states and locally orthogonal triples $A \perp A' \perp A''$, $B \perp B' \perp B''$:

$$
\begin{aligned}
&\langle AB' + A'B\rangle_\rho^2 + \langle AB - A'B'\rangle_\rho^2 \\
&\quad \leqslant \left(1 - \langle A''\rangle_\rho^2\right)\left(1 - \langle B''\rangle_\rho^2\right).
\end{aligned} \tag{7}
$$

Clearly, the right-hand side of this inequality is bounded by 1. However, as noted before, entangled states can saturate inequality (3)—even for orthogonal observables—and attain the value of 4 for the left-hand side and thus clearly violate the bound (7). In contrast to (3), inequality (7) thus does provide a criterion for testing entanglement. The strength of this bound for entanglement detection in comparison with the traditional Bell–CHSH inequality (1) may be illustrated by considering the region of values it allows in the $(\langle X\rangle_\rho, \langle Y\rangle_\rho)$-plane, where $\langle X\rangle_\rho = \langle AB - A'B'\rangle_\rho$ and $\langle Y\rangle_\rho = \langle AB' + A'B\rangle_\rho$, cf. Fig. 1. Note that even in the weakest case (i.e., if $\langle A''\rangle_\rho = \langle B''\rangle_\rho = 0$), it wipes out just over 60% of the area allowed by inequality (1). This quadratic inequality even implies a strengthening of the Bell–CHSH inequality (1) by a factor $\sqrt{2}$:

$$
\left|\langle AB + AB' + A'B - A'B'\rangle_\rho\right| \leqslant \sqrt{2}, \tag{8}
$$

recently obtained by Roy [22]. In fact, even if one chooses only one pair (say B, B') orthogonal, and let A, A' be arbitrary, one would obtain an upper bound of 2 in (7), and still improve upon the Bell–CHSH inequality. Another pleasant feature of inequality (7) is that for pure states its violation is a necessary and sufficient condition for entanglement (see Appendix A). Also, for future purposes we note that the expression in left-hand side is invariant under rotations of A, A' around the axis A'' and rotations of B, B' around B''.

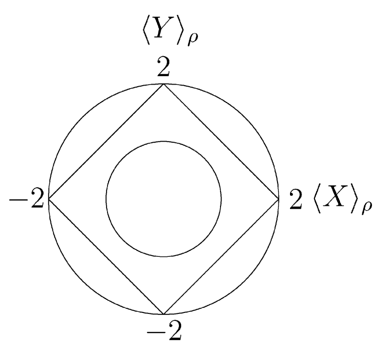

Fig. 1. Comparing the regions in the $(\langle X\rangle, \langle Y\rangle)$-plane allowed (i) by inequality (3) which holds for all quantum states (the inside of the large circle); (ii) by the Bell-CHSH inequality (1) (the inside of the square); and (iii) by the strengthened inequality (7) which holds for all separable quantum states (inside the inner circle with radius 1).

The inequalities (7) present a necessary criterion for a quantum state to be separable—and its violation thus a sufficient criterion for entanglement—but in contrast to pure states, they are clearly not sufficient for separability of mixed states. In Section 4 we shall present an even stronger set of inequalities that is necessary and sufficient for mixed states as well, but we will first discuss the results obtained so far in the light of LHV theories.

3. Comparison to local hidden-variable theories

It is interesting to ask whether one can obtain a similar stronger inequality as (7) in the context of local hidden-variable theories. It is well known that inequality (1) holds also for any such theory in which dichotomous outcomes $a, b \in \{+, -\}$ are subjected to a probability distribution

$$
p(a, b) = \int_\Lambda d\lambda\, \rho(\lambda) P_{\boldsymbol{a}}(a|\lambda) P_{\boldsymbol{b}}(b|\lambda). \tag{9}
$$

Here, $\lambda \in \Lambda$ denotes the "hidden variable", $\rho(\lambda)$ denotes a probability density over Λ, $\boldsymbol{a}$ and $\boldsymbol{b}$ denote the 'parameter settings', i.e., the directions of the spin components measured, and $P_{\boldsymbol{a}}(a|\lambda)$, $P_{\boldsymbol{b}}(b|\lambda)$ are the probabilities (given λ) to obtain outcomes a and b when measuring the settings $\boldsymbol{a}$ and $\boldsymbol{b}$, respectively. The locality condition is expressed by the factorization condition $P_{\boldsymbol{a},\boldsymbol{b}}(a, b|\lambda) = P_{\boldsymbol{a}}(a|\lambda) P_{\boldsymbol{b}}(b|\lambda)$.

The assumption to be added to such an LHV theory in order to obtain the strengthened inequality (7) is the requirement that for any orthogonal choice of A, A' and A'' and for every given λ we have

$$
\langle A\rangle_\lambda^2 + \langle A'\rangle_\lambda^2 + \langle A''\rangle_\lambda^2 = 1, \tag{10}
$$

or at least

$$
\langle A\rangle_\lambda^2 + \langle A'\rangle_\lambda^2 \leqslant 1, \tag{11}
$$

where $\langle A\rangle_\lambda = \sum_{a=\pm 1} a P_{\boldsymbol{a}}(a|\lambda)$, etc.

But a requirement like (10) or (11) is by no means obvious for a local hidden-variable theory. Indeed, as has often been pointed out, such a theory may employ a mathematical framework which is completely different from quantum theory. There is no *a priori* reason why the orthogonality of spin directions should have any particular significance in the hidden-variable theory, and why such a theory should conform to quantum mechanics in reproducing (11) if one conditionalizes on a given hidden-variable state. (One is reminded here of Bell's critique [23] of von Neumann's 'no-go' theorem.) Indeed, (11) is violated by Bell's own example of an LHV model [3] and in fact it must fail in every deterministic LHV theory (where all probabilities $P_{\boldsymbol{a}}(a|\lambda)$, $P_{\boldsymbol{b}}(b|\lambda)$ are either 0 or 1), since for those theories $\langle A\rangle_\lambda^2 = \langle A'\rangle_\lambda^2 = \langle A''\rangle_\lambda^2 = 1$. Thus, the additional requirement (11) would appear entirely unmotivated within an LHV theory.

It thus appears that testing for entanglement within quantum theory and testing quantum mechanics against the class of all LHV theories are not equivalent issues. Of course, this conclusion is not new. Werner [12] has already constructed an explicit LHV model for a specific entangled state. Consider the so-called Werner states: $\rho_W = \frac{1-p}{4}\mathbb{1} + p|\psi^-\rangle\langle\psi^-|$, $p \in [0,1]$. Werner showed [12] that these states are entangled if $p > 1/3$, but nevertheless possess an LHV model for $p = 1/2$. The above inequality (7) suggests that the phenomenon exhibited by this Werner state is much more ubiquitous, i.e., that many more entangled states have an LHV model. We will show that this is indeed the case.

It is not easy to find the general set of quantum states that possess an LHV model [12,24]. Certainly, the question cannot be decided by considering orthogonal observables only. However, as shown in Appendix B, it is possible to determine the class of states for which

$$\max_{A\perp A', B\perp B'} \langle AB' + A'B\rangle_\rho^2 + \langle AB - A'B'\rangle_\rho^2 > 1 \tag{12}$$

holds (they are thus entangled), and which in addition satisfy the Bell–CHSH inequalities of Eq. (1) for *all* choices of observables, i.e., not restricted to orthogonal directions.

Since the latter are known [25–28] to form a necessary and sufficient set of conditions for the existence of an LHV model for all standard Bell experiments on spin-1/2 particles, we conclude that all correlations obtained from such entangled states can be reconstructed by an LHV model.[1] It follows from Appendix B that this class of states includes the Werner states for the region $1/2 < p \leqslant 1/\sqrt{2}$, which complements results obtained by Ref. [5] in which the non-existence of an LHV model is demonstrated for $1/\sqrt{2} < p \leqslant 1$.

4. A necessary and sufficient condition for separability

The inequalities (7) can be strengthened even further. To see this it is useful to introduce, for some given pair of locally orthogonal triples (A, A', A'') and (B, B', B''), eight new two qubit operators on $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$:

$$\begin{aligned}
I &:= \frac{1}{2}(\mathbb{1} + A''B''), & \tilde{I} &:= \frac{1}{2}(\mathbb{1} - A''B''),\\
X &:= \frac{1}{2}(AB - A'B'), & \tilde{X} &:= \frac{1}{2}(AB + A'B'),\\
Y &:= \frac{1}{2}(A'B + AB'), & \tilde{Y} &:= \frac{1}{2}(A'B - AB'),\\
Z &:= \frac{1}{2}(A'' + B''), & \tilde{Z} &:= \frac{1}{2}(A'' - B''),
\end{aligned} \tag{13}$$

[1] Note that experiments with more general measurement scenarios (e.g., collective, sequential or postselected measurements) might still produce correlations incompatible with any LHV model. However, we will not discuss this issue.

where $\frac{1}{2}(A'' + B'')$ is shorthand for $\frac{1}{2}(A'' \otimes \mathbb{1} + \mathbb{1} \otimes B'')$, etc. Note that $X^2 = Y^2 = Z^2 = I^2 = I$ and similar for their tilde versions, and that all eight operators mutually anti-commute. Furthermore, if the orientations of the two triples is the same (e.g., $[A, A'] = 2iA''$ and $[B, B'] = 2iB''$), they form two representations of the generalized Pauli-group, i.e., they have the same commutation relations as the Pauli matrices on $\mathbb{C}^2$, i.e., $[X, Y] = 2iZ$, etc., and $\langle X\rangle_\rho^2 + \langle Y\rangle_\rho^2 + \langle Z\rangle_\rho^2 \leqslant \langle I\rangle^2$ with equality only for pure states (analogous for the tilde version). Note that these two sets transform in each other by replacing $B' \to -B'$ and $B'' \to -B''$.

Now we can repeat the argument of Section 2. Let us first temporarily assume the state to be pure and separable, $|\Psi\rangle = |\psi\rangle|\phi\rangle$. We then obtain:

$$\begin{aligned}
\langle X\rangle_\Psi^2 + \langle Y\rangle_\Psi^2 &= \frac{1}{4}\big(\langle AB - A'B'\rangle_\Psi^2 + \langle A'B + AB'\rangle_\Psi^2\big)\\
&= \frac{1}{4}\big(\langle A\rangle_\psi^2 + \langle A'\rangle_\psi^2\big)\big(\langle B\rangle_\phi^2 + \langle B'\rangle_\phi^2\big)\\
&= \langle \tilde{X}\rangle_\Psi^2 + \langle \tilde{Y}\rangle_\Psi^2
\end{aligned} \tag{14}$$

and similarly:

$$\begin{aligned}
\langle I\rangle_\Psi^2 - \langle Z\rangle_\Psi^2 &= \frac{1}{4}\big(\langle 1 + A''B''\rangle_\Psi^2 - \langle A'' + B''\rangle_\Psi^2\big)\\
&= \frac{1}{4}\big(1 - \langle A''\rangle_\psi^2\big)\big(1 - \langle B''\rangle_\phi^2\big)\\
&= \langle \tilde{I}\rangle_\Psi^2 - \langle \tilde{Z}\rangle_\Psi^2.
\end{aligned} \tag{15}$$

In view of (5) we conclude that for all pure separable states all expressions in Eqs. (14) and (15) are equal to each other. Of course, this conclusion does not hold for mixed separable states. However, $\sqrt{\langle X\rangle_\rho^2 + \langle Y\rangle_\rho^2}$ and $\sqrt{\langle \tilde{X}\rangle_\rho^2 + \langle \tilde{Y}\rangle_\rho^2}$ are convex functions of ρ whereas the three expressions $\sqrt{\langle I\rangle_\rho^2 - \langle Z\rangle_\rho^2}$, $\frac{1}{4}\sqrt{(1 - \langle A''\rangle_\rho^2)(1 - \langle B''\rangle_\rho^2)}$ and $\sqrt{\langle \tilde{I}\rangle_\rho^2 - \langle \tilde{Z}\rangle_\rho^2}$ are all concave in ρ. Therefore we can repeat a similar chain of reasoning as in (6) to obtain the following inequalities, which are valid for all mixed separable states:

$$\left.\begin{aligned}\langle X\rangle_\rho^2 + \langle Y\rangle_\rho^2\\ \langle \tilde{X}\rangle_\rho^2 + \langle \tilde{Y}\rangle_\rho^2\end{aligned}\right\} \leqslant \begin{cases}\langle \tilde{I}\rangle_\rho^2 - \langle \tilde{Z}\rangle_\rho^2,\\ \frac{1}{4}(1 - \langle A''\rangle_\rho^2)(1 - \langle B''\rangle_\rho^2),\\ \langle I\rangle_\rho^2 - \langle Z\rangle_\rho^2.\end{cases} \tag{16}$$

This result extends the previous inequality (7). The next obvious question is then which of the three right-hand sides in (16) provides the lowest upper bound. It is not difficult to show that the ordering of these three expressions depends on the correlation coefficient $C_\rho = \langle A''B''\rangle_\rho - \langle A''\rangle_\rho\langle B''\rangle_\rho$. A straightforward calculation shows that if $C_\rho \geqslant 0$,

$$\begin{aligned}
\langle I\rangle_\rho^2 - \langle Z\rangle_\rho^2 &\leqslant \frac{1}{4}\big(1 - \langle A''\rangle_\rho^2\big)\big(1 - \langle B''\rangle_\rho^2\big)\\
&\leqslant \langle \tilde{I}\rangle_\rho^2 - \langle \tilde{Z}\rangle_\rho^2
\end{aligned} \tag{17}$$

while the above inequalities are inverted when $C_\rho \leqslant 0$. Hence, depending on the sign of C_ρ, either $\langle I\rangle_\rho^2 - \langle Z\rangle_\rho^2$ or $\langle \tilde{I}\rangle_\rho^2 - \langle \tilde{Z}\rangle_\rho^2$ yields the sharper upper bound. In other words, for all separable quantum states one has:

$$\left.\begin{aligned}\langle X\rangle_\rho^2+\langle Y\rangle_\rho^2\\ \langle\tilde X\rangle_\rho^2+\langle\tilde Y\rangle_\rho^2\end{aligned}\right\}\leqslant\left\{\begin{aligned}&\langle\tilde I\rangle_\rho^2-\langle\tilde Z\rangle_\rho^2,\\ &\langle I\rangle_\rho^2-\langle Z\rangle_\rho^2.\end{aligned}\right. \tag{18}$$

This set of inequalities provides the announced strengthening of (7). This improvement pays off: in contrast to (7), the validity of the inequalities (18) for all orthogonal triples A, A', A'' and B, B', B'' provides a necessary and sufficient condition for separability for all states pure or mixed. (See Appendix C for a proof.)

We note that a special case of the inequalities (18), to wit

$$\langle\tilde X\rangle_\rho^2+\langle\tilde Y\rangle_\rho^2\leqslant\langle I\rangle_\rho^2-\langle Z\rangle_\rho^2 \tag{19}$$

was already found by Yu et al. [7], by a rather different argument. These authors stressed that the orientation of the locally orthogonal observables play a crucial role in this inequality: if one chooses both triples to have a *different* orientation (i.e., $A=i[A',A'']/2$ and $B=-i[B',B'']/2$ or $A=-i[A',A'']/2$ and $B=i[B',B'']/2$) the inequality (19) holds trivially for all quantum states ρ, whether entangled or not. It is only when the orientation between those two triples is *the same* that inequality (19) can be violated by entangled quantum states.

The present result (18) complements their findings by showing that the relative orientation of the two triples is not a crucial factor in entanglement detection. Instead, if the orientations are the same, both of the following inequalities contained in (18)

$$\langle X\rangle_\rho^2+\langle Y\rangle_\rho^2\leqslant\langle\tilde I\rangle_\rho^2-\langle\tilde Z\rangle_\rho^2, \tag{20}$$

$$\langle\tilde X\rangle_\rho^2+\langle\tilde Y\rangle_\rho^2\leqslant\langle I\rangle_\rho^2-\langle Z\rangle_\rho^2 \tag{21}$$

are useful tests for entanglement, while the remaining two become trivial. If on the other hand, the orientations are opposite, their role is taken over by

$$\langle X\rangle_\rho^2+\langle Y\rangle_\rho^2\leqslant\langle I\rangle_\rho^2-\langle Z\rangle_\rho^2, \tag{22}$$

$$\langle\tilde X\rangle_\rho^2+\langle\tilde Y\rangle_\rho^2\leqslant\langle\tilde I\rangle_\rho^2-\langle\tilde Z\rangle_\rho^2 \tag{23}$$

while (20) and (21) hold trivially.

5. Experimental aspects of the new inequalities

In this section we compare the strength of the inequalities (18) to some other experimentally feasible criteria to distinguish separable and entangled two qubit states that are not based on Bell-type inequalities. Also, we discuss the problem of whether a finite set of triples for the inequalities (18) could be necessary and sufficient for separability.

A well-known alternative criterion for separability is the fidelity criterion, which says that for all separable states the fidelity F (i.e., the overlap with a Bell state $|\phi_\alpha^+\rangle=\frac{1}{\sqrt2}(|\uparrow\uparrow\rangle+e^{i\alpha}|\downarrow\downarrow\rangle)$, $\alpha\in\mathbb{R}$) is bounded as

$$\begin{aligned}F(\rho)&:=\max_\alpha\langle\phi_\alpha^+|\rho|\phi_\alpha^+\rangle\\ &=\frac12\big(\langle\uparrow\uparrow|\rho|\uparrow\uparrow\rangle+\langle\downarrow\downarrow|\rho|\downarrow\downarrow\rangle\big)+|\rho_\nearrow|\leqslant\frac12.\end{aligned} \tag{24}$$

Here, $\rho_\nearrow$ denotes the extreme anti-diagonal element of ρ, i.e., $\rho_\nearrow=\langle\uparrow\uparrow|\rho|\downarrow\downarrow\rangle$. For a proof, see [8]. An equivalent formulation of (24), using $\operatorname{Tr}\rho=1$ is

$$2|\rho_\nearrow|\leqslant\langle\uparrow\downarrow|\rho|\uparrow\downarrow\rangle+\langle\downarrow\uparrow|\rho|\downarrow\uparrow\rangle. \tag{25}$$

However, choosing the standard Pauli matrices for both triples, i.e. $(A,A',A'')=(B,B',B'')=(\sigma_x,\sigma_y,\sigma_z)$ we obtain from (18)

$$\begin{aligned}&\langle X\rangle^2+\langle Y\rangle^2\leqslant\langle\tilde I\rangle_\rho^2-\langle\tilde Z\rangle_\rho^2\\ &\quad\Longleftrightarrow 4|\rho_\nearrow|^2\leqslant\big(\langle\uparrow\downarrow|\rho|\uparrow\downarrow\rangle+\langle\downarrow\uparrow|\rho|\downarrow\uparrow\rangle\big)^2\\ &\qquad\qquad-\big(\langle\uparrow\downarrow|\rho|\uparrow\downarrow\rangle-\langle\downarrow\uparrow|\rho|\downarrow\uparrow\rangle\big)^2\end{aligned} \tag{26}$$

which implies (25). Clearly, then, (18) is stronger than the fidelity criterion, i.e., it will detect more entangled states.

As another application, consider the following entanglement witnesses for so-called local orthogonal observables (LOOs) $\{G_k^A\}_{k=1}^4$ and $\{G_k^B\}_{k=1}^4$: a linear one presented by [9]:

$$\langle\mathcal{W}\rangle_\rho=1-\sum_{k=1}^4\langle G_k^A\otimes G_k^B\rangle_\rho, \tag{27}$$

and a nonlinear witness from [10] given by

$$\begin{aligned}\mathcal{F}(\rho)=1&-\sum_{k=1}^4\langle G_k^A\otimes G_k^B\rangle_\rho\\ &-\frac12\sum_{k=1}^4\langle G_k^A\otimes\mathbb{1}-\mathbb{1}\otimes G_k^B\rangle_\rho^2.\end{aligned} \tag{28}$$

Here, the set $\{G_k^A\}_{k=1}^4$ is a set of four observables that form a basis for all operators in the Hilbert space of a single qubit and which satisfy orthogonality relations $\operatorname{Tr}[G_kG_{k'}]=\delta_{kk'}$ $(k,k'=1,\dots,4)$. A typical complete set of LOOs is formed by any orthogonal triple of spin directions conjoined with the identity operator, i.e., in the notation of this Letter, $\{G_k^A\}_{k=1}^4=\{\mathbb{1},A,A',A''\}/\sqrt2$ and similarly for $\{G_k^B\}_{k=1}^4$.

These witnesses provide tests for entanglement in the sense that for all separable states $\langle\mathcal{W}\rangle_\rho\geqslant0$, $\mathcal{F}(\rho)\geqslant0$ must hold and a violation of either of these inequalities is thus a sufficient condition for entanglement. An optimization procedure for the choice of LOOs in these two witnesses is given in Ref. [11].

The strength of these two criteria has been studied for the noisy singlet state introduced in Ref. [10]: $\rho=p|\psi^-\rangle\langle\psi^-|+(1-p)\rho_{\text{sep}}$, where $|\psi^-\rangle=(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)/\sqrt2$ is the singlet state and the separable noise is $\rho_{\text{sep}}=2/3|\uparrow\uparrow\rangle\langle\uparrow\uparrow|+1/3|\uparrow\downarrow\rangle\langle\uparrow\downarrow|$. The Peres–Horodecki criterion [29] gives that this state ρ is entangled for any $p>0$. Under the complete set of LOOs $\{-\sigma_x,-\sigma_y,-\sigma_z,\mathbb{1}\}^A/\sqrt2$, $\{\sigma_x,\sigma_y,\sigma_z,\mathbb{1}\}^B/\sqrt2$, the linear witness given above can detect the entanglement for all $p>0.4$ [11], and the nonlinear one detects the entanglement for $p>0.25$ [10]. Using the optimization procedure of Ref. [11] the optimal choice of LOOs for the linear witness can detect the entanglement for all $p>0.292$, whereas the nonlinear witness appears to be already optimal.

Using the same set of LOOs as above, the quadratic separability inequality (18) detects the entanglement already for $p>0$

(i.e., as soon as the state is entangled it can be detected), and it is thus stronger than these two witnesses for this particular state.

As a final topic, we wish to point out that, in spite of the strength of the inequalities (18) as a necessary and sufficient condition for separability, they also have an important drawback from an experimental point of view. In order to check their validity or violation one would have to measure for *all* locally orthogonal triples of observables, a task which is obviously unfeasible since there are uncountably many of those. Because of this one must generally gather some prior knowledge about the state whose entanglement is to be detected, so that one can choose settings that allow for a violation. It is therefore highly interesting to ask whether a finite collection of orthogonal triples could be found for which the satisfaction of these inequalities would already provide a necessary and sufficient condition for separability, since then such prior knowledge would no longer be necessary. Measuring the finite collection of settings would then be always sufficient for entanglement detection, independent of the state to be detected.

We have performed an (unsystematic) survey of this problem. A first natural attempt would be to consider the triples obtained by permutations of the basis vectors. Thus, consider the set of three inequalities obtained by taking for both triples (A, A', A'') and (B, B', B'') the choices $\alpha = (\sigma_x, \sigma_y, \sigma_z)$, $\beta = (\sigma_z, \sigma_y, \sigma_x)$ and $\gamma = (\sigma_z, \sigma_x, \sigma_y)$. (Other permutations do not contribute independent inequalities.)

Under this choice, (18) leads to the six inequalities

$$\langle X_k\rangle^2 + \langle Y_k\rangle^2 \leqslant \langle \tilde{I}_k\rangle^2 - \langle \tilde{Z}_k\rangle^2, \tag{29}$$

$$\langle \tilde{X}_k\rangle^2 + \langle \tilde{Y}_k\rangle^2 \leqslant \langle I_k\rangle^2 - \langle Z_k\rangle^2, \tag{30}$$

for $k = \alpha, \beta, \gamma$.

For a general pure state $|\Psi\rangle = a|{\uparrow\uparrow}\rangle + b|{\uparrow\downarrow}\rangle + c|{\downarrow\uparrow}\rangle + d|{\downarrow\downarrow}\rangle$, the satisfaction of these inequalities boils down to three equations:

$$|ad| = |bc|, \tag{31}$$

$$\left|(a+d)^2 - (b+c)^2\right| = \left|(a-d)^2 - (b-c)^2\right|, \tag{32}$$

$$\left|(b+c)^2 + (a-d)^2\right| = \left|(b-c)^2 + (a+d)^2\right|. \tag{33}$$

However, these equations are satisfied if $a = c = i$, $-b = d = 1$, i.e., for an entangled pure state. This shows that the choice α, β, γ above does not produce a sufficient condition for separability.

However, let us make an amended choice β': take the observables β and apply a rotation U for the observables of particle 1 around the y-axis over 45 degrees, i.e., take $(A, A', A'')_{\beta'} = (U\sigma_z U^\dagger, \sigma_y, U\sigma_x U^\dagger)$ and $(B, B', B'')_{\beta'} = (\sigma_z, \sigma_y, \sigma_x)$; and γ': take the observables of choice γ and apply rotation U on the observables for particle 1 (i.e., over 45 degrees around the y-axis) followed up by rotation V over 45 degrees around the z-axis on the same observables, in other words: $(A, A', A'')_{\gamma'} = (VU\sigma_z U^\dagger V^\dagger, VU\sigma_x U^\dagger V^\dagger, VU\sigma_y U^\dagger V^\dagger)$ and $(B, B', B'')_{\gamma'} = (\sigma_z, \sigma_x, \sigma_y)$.

The choice α, β' and γ' gives for the above arbitrary pure state $|\Psi\rangle$:

$$|ad| = |bc|, \tag{34}$$

$$\left|(a+c)(b-d)\right| = \left|(a-c)(b+d)\right|, \tag{35}$$

$$\left|(a+ic)(b-id)\right| = \left|(a-ic)(b+id)\right|. \tag{36}$$

A tedious but straightforward calculation shows that these equations are fulfilled *only* if $ad = bc$, i.e., if $|\Psi\rangle$ is separable. Hence, by measuring the observables in the directions indicated by the choice α, β' and γ', the inequalities (18) do provide a necessary and sufficient criterion for separability for pure states. We have not been able to check whether this result extends to mixed states.

6. Conclusion

It has been shown that for two spin-1/2 particles (qubits) and orthogonal spin components quadratic separability inequalities hold that impose much tighter bounds on the correlations in separable states than the traditional Bell–CHSH inequality. In fact, the quadratic inequalities (18) are so strong that their validity for all orthogonal bases is a necessary and sufficient condition for separability of all states, pure or mixed, and a subset of these inequalities for just three orthogonal bases (giving six inequalities) is a necessary and sufficient condition for the separability of all pure states. Furthermore, the orientation of the measurement basis is shown to be irrelevant, which ensures that no shared reference frames needs to be established between the measurement apparata for each qubit.

The quadratic inequalities (18) have been shown to be stronger than both the fidelity criterion and the linear and nonlinear entanglement witnesses based on LOOs as given in [9, 10]. Experimental tests for entangled states using orthogonal directions can therefore be considerably strengthened by means of the quadratic inequalities (18). As we will discuss elsewhere in more detail [30], these inequalities provide tests of entanglement that are much more robust against noise than many alternative criteria. There we will also extend the analysis to the N-qubit case by generalizing the method of Section 4 to more than two qubits.

Furthermore, we have argued that these quadratic Bell inequalities do not hold in LHV theories. This provides a more general example of the fact first discovered by Werner, i.e., that some entangled states do allow an LHV reconstruction for all correlations in a standard Bell experiment. What is more, there appears to be a ‘gap’ between the correlations that can be obtained by separable quantum states and those obtainable by LHV models. This nonequivalence between the correlations obtainable from separable quantum states and from LHV theories means that, apart from the question raised and answered by Bell (can the predictions of quantum mechanics be reproduced by an LHV theory?) it is also interesting to ask whether separable quantum states can reproduce the predictions of an LHV theory. The answer, as we have seen, is negative: quantum theory generally needs entangled states even in order to reproduce the classical correlations of such an LHV theory. In fact, as we will show in forthcoming work [30], the gap between the correlations allowed by local hidden-variable theories and those achievable by separable quantum states increases exponentially with the number of particles.

Appendix A

Here we prove that any pure two-qubit state satisfying (5) must be separable. By the bi-orthogonal decomposition theorem, and following Ref. [4], any pure state can be written in the form $|\Psi\rangle = r|\uparrow\downarrow\rangle - s|\downarrow\uparrow\rangle$, with $r, s \geqslant 0$, $r^2 + s^2 = 1$. For this state $\langle \boldsymbol{a}\cdot\boldsymbol{\sigma} \otimes \boldsymbol{b}\cdot\boldsymbol{\sigma}\rangle_\Psi = -a_z b_z - 2rs(a_x b_x + a_y b_y)$, etc. Using this and choosing $\boldsymbol{a} = (0,0,1)$, $\boldsymbol{a'} = (1,0,0)$ and $\boldsymbol{b} = (\sin\beta, 0, \cos\beta)$, $\boldsymbol{b'} = (-\cos\beta, 0, \sin\beta)$ we obtain $\langle AB' + A'B\rangle^2 + \langle AB - A'B'\rangle^2 = (1+2rs)^2$. If (7) holds, this expression is smaller than or equal to 1, and it follows that $rs = 0$, i.e., the state $|\Psi\rangle$ is not entangled.

Appendix B

Here we provide further examples of entangled states that satisfy the Bell–CHSH inequalities (1) for all observables in the standard Bell experiment. First note [5] that any two-qubit state can be written in the form $\rho = \frac{1}{4}(\mathbb{1}\otimes\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma}\otimes\mathbb{1} + \mathbb{1}\otimes\boldsymbol{s}\cdot\boldsymbol{\sigma} + \sum_{ij=1}^{3} t_{ij}\sigma_i\otimes\sigma_j)$, where $\boldsymbol{r} = \mathrm{Tr}\,\rho(\boldsymbol{\sigma}\otimes\mathbb{1})$, $\boldsymbol{s} = \mathrm{Tr}\,\rho(\mathbb{1}\otimes\boldsymbol{\sigma})$ and $t_{ij} = \mathrm{Tr}\,\rho(\sigma_i\otimes\sigma_j)$. By employing the freedom of choosing local coordinate frames at both sites separately, we can bring the matrix (t_{ij}) to diagonal form [31], i.e., $t = \mathrm{diag}(t_{11}, t_{22}, t_{33})$, and arrange that $t_{ii} \geqslant 0$. Furthermore, since the labelling of the coordinate axes is arbitrary, we can also pick an ordering such that $t_{11} \geqslant t_{22} \geqslant t_{33}$.

Now let α, α', β, β' denote two pairs of arbitrary spin observables, for particle 1 and 2 respectively, $\alpha = \boldsymbol{\alpha}\cdot\boldsymbol{\sigma}\otimes\mathbb{1}$, $\beta = \mathbb{1}\otimes\boldsymbol{\beta}\cdot\boldsymbol{\sigma}$ and similar for the primed observables. It is easy to see that the maximum of $|\langle\alpha\beta + \alpha\beta' + \alpha'\beta - \alpha'\beta'\rangle_\rho|$ for all choices of observables will be attained by taking the vectors $\boldsymbol{\alpha}, \boldsymbol{\alpha'}, \boldsymbol{\beta}, \boldsymbol{\beta'}$ coplanar,[2] and in fact, in the plane spanned by the two eigenvectors of t with the largest eigenvalues, i.e., t_{11} and t_{22}. As shown by Ref. [5], this maximum is $\max_{\alpha,\beta,\alpha',\beta'} |\langle\alpha\beta + \alpha\beta' + \alpha'\beta - \alpha'\beta'\rangle_\rho| = 2\sqrt{t_{11}^2 + t_{22}^2}$. Thus ρ will satisfy all Bell–CHSH inequalities if $t_{11}^2 + t_{22}^2 \leqslant 1$, which is the necessary and sufficient condition for the existence of an LHV model [26].

Now consider the maximum of $\langle AB - A'B'\rangle_\rho^2 + \langle AB' + A'B\rangle_\rho^2$, with $A \perp A'$ and $B \perp B'$. Clearly, these spin observables should be chosen in the same plane as before, spanned by the eigenvectors corresponding to t_{11} and t_{22}. As mentioned in the text, the expression is invariant under rotations of A, A' or B, B' in this plane. Choosing $A = B = \sigma_x$, $A' = -B' = \sigma_y$ the maximum is equal to $\max_{A\perp A', B\perp B'}\langle AB - A'B'\rangle^2 + \langle AB' + A'B\rangle^2 = (t_{11} + t_{22})^2$. Clearly, state ρ will be both entangled and satisfy all Bell–CHSH inequalities for all observables (and thus allow for an LHV description) if $t_{11} + t_{22} > 1$ and $t_{11}^2 + t_{22}^2 \leqslant 1$.

[2] Here 'coplanar' refers to a single plane in the local frames of reference. Since these frames may have a different orientation, this does not necessarily refer to a single plane in real space.

Appendix C

Here we will prove that any state ρ that satisfies the inequalities (18) for all orthogonal triples A, A', A'', and B, B', B'' must be separable (the converse has already been proven above).

We proceed from the well-known Peres–Horodecki lemma [29] that a state of two qubits is separable iff $\rho^{\mathrm{PT}} \geqslant 0$ where 'PT' denotes partial transposition. Equivalently, the state is entangled iff, for all pure states $|\Psi\rangle$:

$$\langle\Psi|\rho^{\mathrm{PT}}|\Psi\rangle = \mathrm{Tr}\,\rho^{\mathrm{PT}}|\Psi\rangle\langle\Psi| = \mathrm{Tr}\,\rho\big(|\Psi\rangle\langle\Psi|\big)^{\mathrm{PT}} \geqslant 0. \tag{C.1}$$

We shall show that (C.1) holds whenever ρ obeys (19). Indeed, according to the biorthonormal decomposition theorem (cf. [4]), we can find bases $|\uparrow\rangle, |\downarrow\rangle$ on $\mathcal{H}_1$ and $|\uparrow\rangle, |\downarrow\rangle$ on $\mathcal{H}_2$ such that $|\Psi\rangle = \sqrt{p}|\uparrow\downarrow\rangle + \sqrt{1-p}|\downarrow\uparrow\rangle$. Choosing these bases to be the eigenvectors of A'' and B'' respectively, we thus find

$$|\Psi\rangle\langle\Psi| = \frac{1}{2}\tilde{I} + \left(p - \frac{1}{2}\right)\tilde{Z} + \sqrt{p(1-p)}\tilde{X},$$

$$|\Psi\rangle\langle\Psi|^{\mathrm{PT}} = \frac{1}{2}\tilde{I} + \left(p - \frac{1}{2}\right)\tilde{Z} + \sqrt{p(1-p)}X. \tag{C.2}$$

Hence

$$\langle\Psi|\rho^{\mathrm{PT}}|\Psi\rangle = \frac{1}{2}\langle\tilde{I}\rangle + \left(p - \frac{1}{2}\right)\langle\tilde{Z}\rangle + \sqrt{p(1-p)}\langle X\rangle, \tag{C.3}$$

where the last two terms can be bounded by a Schwartz inequality to yield

$$\left|\left(p - \frac{1}{2}\right)\langle\tilde{Z}\rangle + \sqrt{p(1-p)}\langle X\rangle\right| \leqslant \frac{1}{2}\sqrt{\langle\tilde{Z}\rangle^2 + \langle X\rangle^2} \tag{C.4}$$

and we find $\langle\Psi|\rho^{\mathrm{PT}}|\Psi\rangle \geqslant \frac{1}{2}\langle\tilde{I}\rangle - \frac{1}{2}\sqrt{\langle\tilde{Z}\rangle^2 + \langle X\rangle^2}$. But (19) demands $\langle X\rangle_\rho^2 + \langle\tilde{Z}\rangle_\rho^2 \leqslant \langle\tilde{I}\rangle_\rho^2$ from which it follows that

$$\langle\Psi|\rho^{\mathrm{PT}}|\Psi\rangle \geqslant 0 \tag{C.5}$$

so that the state ρ is separable.

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