Local Hidden Variable Theories for Quantum States

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While all bipartite pure entangled states violate some Bell inequality, the relationship between entanglement and non-locality for mixed quantum states is not well understood. We introduce a simple and efficient algorithmic approach for the problem of constructing local hidden variable theories for quantum states. The method is based on constructing a so-called symmetric quasi-extension of the quantum state that gives rise to a local hidden variable model with a certain numbers of settings for the observers Alice and Bob. We use this method to analytically construct local hidden variable theories for any bound entangled state based on a real unextendible product basis (UPB) with two measurement settings for Alice and Bob. The problem can be approached by semi-definite programming and we present our numerical and analytical results for various classes of states.

It was John Bell [1] who quantified how measurements on entangled quantum mechanical systems can invalidate local classical models of reality. His original inequality has generated a field of research devoted to general Bell inequalities and experimentally observed violations of such inequalities.

Perhaps surprisingly, the nature of the set of states that violate local realism is poorly understood, although it is known from the seminal work of Werner [2] that not all entangled states violate a Bell inequality. Recent results in quantum information theory have revealed the complex structure of the set of entangled states but have as yet shed little light on the relation between this structure and violation of Bell inequalities. For example, it has been conjectured by Peres [3] that so-called bound entangled states which satisfy the Peres-Horodecki “partial transposition” criterion [4] do not violate any Bell inequalities. There are various results that support this conjecture both in the bipartite and multipartite case, see Refs. [5, 6, 7, 8, 9, 10], but none of the results is conclusive. What has been lacking in the literature so far is a systematic way of deciding whether a quantum state does or does not violate some Bell inequality. The difficulty is that the possible types of local measurements and the number of measurements that observers can perform is in principle unbounded and the enumeration of Bell inequalities is computationally hard [11].

In this Letter we present the first systematic approach for constructing local hidden variable theories for quantum states, depending only on the number of local measurement settings for each observer. Our approach has yielded both numerically constructed local hidden variable theories for a variety of quantum states as well as analytical results for Werner states [3] and a class of bound entangled states based on real UPBs [2].

Before we can state our main result, we recapitulate the mathematics of local hidden variable (LHV) models and Bell inequalities for bipartite systems [12]. We refer the reader to Ref. [3, 11, 13] for some literature on the theoretical formulation of general Bell inequalities. Each of the observers, Alice and Bob, has a set of local measurements. Let \( i = 1, \ldots, s_a \) be the number of measurements for Alice and let each measurement have \( o_a(i) \) outcomes. Let \( k = 1, \ldots, s_b \) be the number of measurements for Bob and \( o_b(k) \) be the number of outcomes per measurement. The probability \( P_{ij,kl} \) denotes the probability that Alice’s \( i \)th measurement has outcome \( j \) and Bob’s \( k \)th measurement has outcome \( l \). A local hidden variable model assumes the existence of a shared random variable between Alice and Bob that is used to locally generate a measurement outcome depending only on the choice of the local measurement (and not on the choice of the other, remote, measurement). The local hidden variable model generates the probability vector \( \vec{P} \) with entries \( P_{ij,kl} \) when it generates measurement outcomes in accordance with these probabilities. Mathematically one defines a convex set \( S(s_a, s_b, o_a, o_b) \) which is the set of probability vectors \( \vec{P} \) that can be generated by LHV models. It is known that \( S \) is a polytope and that the extremal vectors \( \vec{B} \) of \( S \) are vectors with 0, 1 entries [3]. For more information on polytopes, see for example [4]. These extremal vectors \( \vec{B} \) correspond to the situation in which the outcomes of the measurements are determined with certainty and can be labelled by 2 sets of indices \( m = (m_1, \ldots, m_{s_a}) \) where \( m_i = 1, \ldots, o_a(i) \) and \( n = (n_1, \ldots, n_{s_b}) \) where \( n_k = 1, \ldots, o_b(k) \). A brief expression for these extremal vectors is

\[
P_{ij,kl}^{m,n} = \delta_{jm_i} \delta_{kn_k}. \tag{1}
\]

In words, each extremal vector specifies a single outcome with probability one for each local measurement, independently of the measurement made by the other parties. An example of an extremal vector for \( s_a = s_b = 2 \) and \( o_a = o_b = 3 \) is given in Table I.

For a quantum mechanical system \( \rho \) in \( \mathcal{H}_{d_A} \otimes \mathcal{H}_{d_B} \) the probability \( P_{ij,kl}(\rho) \) is given by \( P_{ij,kl}(\rho) = \text{Tr} E_{ij}^A \otimes E_{kl}^B(\rho) \).
Here \( \{ E_{ij}^A \geq 0 : \sum_j E_{ij}^A = I_{d_A} \} \) are the POVM elements for Alice’s \( i \)th measurement and \( \{ E_{kl}^B \} \) are the POVM elements for Bob’s \( k \)th measurement. There is a violation of a Bell inequality if and only if \( P_{ij,kl} \) cannot be generated by a LHV model, or \( \tilde{P} \not\in S \).

|   | \( B_1 \) | \( B_2 \) |
|---|---|---|
|   | 1 2 3 | 1 2 3 |
| \( A_1 \) | 1 0 0 | 0 1 0 |
| \( A_2 \) | 0 0 0 | 0 0 0 |
|   | 0 0 0 | 0 1 0 |

TABLE I: An example of an extremal B-vector for 2 settings for Alice and Bob with 3 outcomes per setting.

In this Letter we will prove the first necessary condition for a state to violate a Bell inequality depending only on the number of settings for Alice and Bob. We will explicitly construct a LHV model in a \( (s_a = 2, s_b = 2) \) setting for any bound entangled state based on a real unextendible product basis. Then we will discuss numerical work that shows that many of the known bipartite bound entangled states cannot violate a Bell inequality with two settings for Alice and Bob. Finally, we will partially reproduce and extend some of Werner’s original results by showing that it is possible to use our procedure to analytically construct LHV theories for Werner states. It is noteworthy to mention that our methods (Theorem 1 and Theorem 2) straightforwardly generalize to multipartite states, even though we have not explored this direction.

We will connect violations of Bell inequalities to the existence of a symmetric (quasi-) extension of a quantum state. An extension of a quantum state \( \rho \) on, say, a system \( AB \), is another quantum state defined on a system \( ABC \) such that when we trace over \( C \) we obtain the original quantum state \( \rho \). We are interested in the situation where the system \( C = A^{\otimes(s_a-1)} \otimes B^{\otimes(s_b-1)} \) and we will demand that the extension be invariant under all permutations of the \( s_a \) copies of system \( A \) among each other and similarly invariant under any permutation of the \( B \) systems. It is clear that if the quantum state \( \rho \) is separable, i.e. \( \rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \otimes (|\phi_i\rangle \langle \phi_i|)_{B} \), such an extension always exists: we just copy the individual product states onto the other spaces:

\[
\rho_{\text{ext}} = \sum_i p_i |\psi_i\rangle \langle \psi_i| \otimes s_a \otimes (|\phi_i\rangle \langle \phi_i|) \otimes s_b. \tag{2}
\]

If the state \( \rho \) is a pure entangled state, then it is also clear that such a symmetric extension cannot exist. The symmetry requirement implies that the pure entangled state \( \rho_{AB} \) must equal \( \rho_{A'B} \) where \( A' \) is another \( A \)-system, which is impossible. In popular terms we may say that pure entanglement is ‘monogamous’, \( B \) cannot be entangled with \( A \) and \( A' \) at the same time. In some sense what we show in this paper is that (1) a violation of a Bell inequality indicates that the entanglement in the quantum state is ‘monogamous’ and (2) there are many mixed entangled states whose entanglement is not monogamous.

Thus the existence of a symmetric extension can be viewed as a separability criterion (see Ref. for a similar but stronger separability criterion where one demands that the symmetric extension has positive partial transposes). For considering Bell inequality violations we generalize our criterion slightly and ask whether a state has a symmetric quasi-extension \( H_\rho \) which is not necessarily positive. In order to define this notion we need the definition of a multi-partite entanglement witness, which is an entanglement witness which can detect any multi-partite entanglement in a state. It has the property that for all states \( |\psi_1, \ldots, \psi_{s_a}, \phi_1, \ldots, \phi_{s_b}\rangle H_\rho |\psi_1, \ldots, \psi_{s_a}, \phi_1, \ldots, \phi_{s_b}\rangle \geq 0 \).

**Definition [Symmetric Quasi-Extension]:** Let \( \pi : \mathcal{H}_{s_a} \to \mathcal{H}_{s_b} \) be a permutation of spaces \( \mathcal{H} \) in \( \mathcal{H}_{s_a} \). We define

\[
\text{Sym}(\rho) = \frac{1}{s!} \sum_\pi \pi \rho \pi^\dagger. \tag{3}
\]

We say that \( \rho \) on \( \mathcal{H}_A \otimes \mathcal{H}_B \) has a \( (s_a, s_b) \)-symmetric quasi-extension when there exists a multi-partite entanglement witness \( H_\rho \) on \( \mathcal{H}_{s_a} \otimes \mathcal{H}_{s_b} \) such that

\[
\text{Tr}_{\mathcal{H}_{s_a} \otimes \mathcal{H}_{s_a-1}, \mathcal{H}_{s_b} \otimes \mathcal{H}_{s_b-1}} H_\rho = \rho \text{ and } \tilde{H}_\rho = \text{Sym}_A \otimes \text{Sym}_B(H_\rho).
\]

The reason for considering such quasi-extensions is clear from the following theorems which are the main results of this Letter.

**Theorem 1:** If \( \rho \) has a \( (s_a, s_b) \)-symmetric quasi-extension then \( \rho \) does not violate a Bell inequality with \( (s_a, s_b) \) settings.

Before proving this theorem, it is important to note the generality of the result; it holds for all possible choices of measurements which includes POVM measurements with an unbounded number of measurement outcomes. We will show below that the quasi-extension of \( \rho \) effectively creates a LHV model for \( \rho \) when Alice and Bob have \( s_a \) and \( s_b \) arbitrary measurements.

**Proof** We prove our theorem by extracting an LHV model from the quasi-extension. The LHV model for \( \rho \) for \( (s_a, s_b) \) settings should reproduce the vector \( P_{ij,kl}(\rho) = \text{Tr} E_{ij}^A \otimes E_{kl}^B \) for all possible choices of POVM measurements \( \{ E_{ij}^A, E_{kl}^B \} \), as a convex combination of the extremal B-vectors, i.e.

\[
P_{ij,kl}(\rho) = \sum_{m,n} p_{m,n}(\{ E_{ij}^A, E_{kl}^B \}, \rho) P_{ij,kl}^{m,n}, \tag{4}
\]

where \( p_{m,n}(\cdot) \geq 0 \). If a symmetric quasi-extension exists for \( \rho \) then \( \text{Tr} E_{ij}^A \otimes E_{kl}^B \rho = \text{Tr} (E_{ij}^A \otimes E_{kl}^B \otimes I) H_\rho \). Using the definition of the B-vectors, the properties of the
POVMs \((\sum_i E_{ij}^A = I_{d_A}, B)\), and the symmetry properties of \(H_P\) it is not hard to verify that
\[
P_{ij,kl}(\rho) = \text{Tr} \, E_{ij}^A \otimes E_{kl}^B \rho = \sum_{m,n} (\text{Tr} \, E_m^A \otimes E_n^B H_P) E_{ij,kl}^{m,n}. \tag{5}
\]
Here \(E_m^A = E_{1m_1}^A \otimes E_{2m_2}^A \otimes \ldots \otimes E_{sm_s}^A\) and similarly for \(E_n^B\). Since \(H_P\) is a quasi-extension \(P_{m,n}(E_{ij}, E_{kl}) \rho = \text{Tr} \, E_m^A \otimes E_n^B H_P \geq 0\), and we have obtained a LHV model.

One way of looking at this result is the following \cite{18}. If \(\rho\) has a symmetric extension \(\hat{\rho}\), then instead of measurement on \(\rho\), Alice and Bob can do measurements on \(\hat{\rho}\). Due to the symmetry Alice can do the first measurement on the first Alice space and the second measurement on the second Alice space etc. But now these measurements are all commuting, and can be considered as one big measurement. But we know that when Alice and Bob each have only a single measurement a LHV model for their measurements exists and thus we have a LHV model for the measurements on \(\rho\). With this picture in mind, it is not hard to understand the following strengthening of our results (see also Ref. \cite{14}):

**Theorem 2:** If \(\rho\) has a \((1, s_0)\)-symmetric quasi-extension then \(\rho\) does not violate a Bell inequality with \(s_0\) settings for Bob and any number of settings for Alice.

**Remark** The theorem also holds when Alice and Bob are interchanged.

**Proof:** The intuition behind this theorem relies on the fact that there are no violations of Bell inequalities when one party has only one measurement setting, thus suggesting that it is unnecessary to extend to copies of Alice’s space as well as Bob’s. Here is the local hidden variable model that we construct from a quasi-extension \(H_P\) on \(H_A \otimes H_B^{\otimes s_0}\). We set
\[
p_{m,n}(\{(E_{ij}, E_{kl}^B)\}, \rho) = \frac{\Pi_{s=1}^n (\text{Tr} \, E_{c_{i,s}}^A \otimes E_{d_{j,s}}^B H_P)}{(\text{Tr} \, I_A \otimes E_n^B H_P)^{s-1}}. \tag{6}
\]
Each \(p_{m,n}\) is nonnegative since \(H_P\) is an entanglement witness. We can substitute this expression in Eq. (3) and verify that we obtain the correct probabilities \(P_{ij,kl}(\rho)\) by using the definition of the B-vectors, the normalization of the POVMs, and the symmetry of \(H_P\) as before. \(\square\)

This method for constructing LHV theories may be implemented both numerically and analytically. Let us first show a simple analytic construction of a \((2, 2)\)-symmetric extension for any bound entangled state based on a real unextendible product basis \cite{15}. Let \(P_{BE} = 1 - \sum_i |a_i, b_i\rangle \langle a_i, b_i|\) be the projector onto such a bound entangled state, where \(|a_i, b_i\rangle = |a_i^*, b_i^*\rangle\) is the real unextendible product basis. Our (unnormalized) extension will be \(|\Psi\rangle_{A_1 B_1} \otimes |\Psi\rangle_{B_1 B_2} - \sum_i |a_i, a_i, b_i, b_i\rangle_{A_1 A_2 B_1 B_2}\) where \(|\Psi\rangle = \sum_i |i\rangle\). It is evident that this extension has the desired symmetry property. It is not hard to verify that by tracing over the systems \(A_2\) and \(B_2\) we obtain \(P_{BE}^2 = P_{BE}\). The existence of a symmetric \((2, 2)\)-extension implies the existence of both \((2, 1)\) and \((1, 2)\)
symmetric extensions for the state by tracing out copies of \(A\) or \(B\), so any Bell inequality violation for this class of states must involve more than two measurement settings for both parties.

We have implemented numerical tests for the conditions of these two theorems. Firstly we look for the existence of a symmetric extension with \(H_P \geq 0\). If such an extension does not exist, there is still the possibility that some other kind of quasi-extension does exist. We have focussed on the existence of a decomposable entanglement witness \(H_P\) because in both these cases the numerical problem corresponds to a semi-definite program \cite{13}. We label the partitions of \(H_A^{\otimes s_a} \otimes H_B^{\otimes s_b}\) into bipartite systems by \(p\) and we denote partial transposition with respect to one of the two subsystems as \(T_p\). A decomposable entanglement witness may then be written as \(H_P = P + \sum_p Q_p^T\) where \(P \geq 0, Q_p \geq 0\) for all \(p\). (In fact, due to the symmetry it is only necessary to include partitions unrelated by permutations of copies of \(A\) or \(B\) in the sum, as in Ref. \cite{16}.)

Semi-definite programs correspond to optimizations of linear functions on positive matrices subject to trace constraints. They are convex optimizations and are particularly tractable both analytically and numerically. We show how to numerically construct symmetric extensions, the decomposable quasi-extension case is very similar. The condition that the partial trace of \(H_P\) is \(\rho\) equivalent to requiring that \(\text{Tr} \, (X \otimes I) H_P = \text{Tr} \, X \rho\) for all operators \(X\) on \(H_A \otimes H_B\). If we write \(X\) in terms of a basis \(\{\sigma_i\}\) for the vector space of operators then by linearity it is enough to check that this trace constraint holds for each element of the basis. We will assume that the basis is orthogonal in the trace inner product \(\text{Tr} \, \sigma_i \sigma_j = \delta_{ij}\) and that \(\sigma_0 = I_{d_A} \otimes I_{d_B}/\sqrt{d_Ad_B}\). The index \(i\) ranges from zero to \((d_Ad_B)^2 - 1\). Consider then this semi-definite program

\[
\begin{array}{ll}
\text{minimize} & \text{Tr} \, K \\
\text{subject to} & \text{Tr} \, \text{Sym}_A \otimes \text{Sym}_B (\sigma_i \otimes I) K = r_i, \quad i > 0, \\
& \text{Tr} \, K \geq 0,
\end{array}
\]

where \(r_i = \text{Tr} \, \sigma_i \rho\). If the optimum is less than or equal to one, then, by adding a multiple of the identity to the optimal \(K\), we obtain some \(K_p\) that satisfies \(\text{Tr} \, K_p = 1\) as well as the other constraints. If we define \(H_P \equiv \text{Sym}_A \otimes \text{Sym}_B(K_p)\) it is clear that \(H_P\) is a \((s_a, s_b)\)-symmetric extension of \(\rho\). Duality properties of semi-definite programs imply that an optimum greater than one precludes the existence of a \((s_a, s_b)\)-symmetric extension \(\Sigma\) (see also the Appendix).

We have implemented this semi-definite program using SeDuMi \cite{16} for several examples of bound entangled states with \(d_A = d_B = 3\). The results are summarized
in Table IV. For (1, 2) settings the extension code took 1–3s to run on a 500 MHz Pentium 3 desktop with 500 MB of RAM, while the quasi-extension code took 1.5–4s. The computation for both forms of the code as described above should scale roughly as $d^2 A + d^2 B = 16$. However as $s_a$ and $s_b$ grow, the permutation symmetry of the extensions can be used to dramatically reduce the size of the problem by block diagonalizing the matrices $\text{Sym}_A \otimes \text{Sym}_B (\sigma_i \otimes I)$ and removing repeated blocks [23, 24]. For a fixed $A, B$ the computation will scale polynomially with $s_a$ and $s_b$. We implemented such a code in the case of (1, 3)-extensions which took 1.5–4s for a single state.

The Choi-Horodecki (C-H) states considered in Ref. [22] depend on a parameter $\alpha$ and include separable ($\alpha \in [2, 3]$), bound entangled ($\alpha \in (3, 4]$) and nonpositive partial transpose states for $\alpha > 4$. They turn out to have (2, 1)-symmetric extensions well into the range for which the states are entangled. Over the range $\alpha \in [4, 34, 84]$ they have decomposable symmetric quasi-extensions but no symmetric extensions showing that the former property provides a strictly stronger sufficient condition for the existence of an LHV theory.

On the other hand, we found that the two parameter family of bound entangled states introduced by Horodecki and Lewenstein [23] do not have (2, 1)-symmetric extensions or quasi-extensions. Also, many of the states described by Bruß and Peres [24] do not appear to possess symmetric quasi-extensions. However, for several examples of these two kinds of states we searched numerically over measurement settings to look for violations of extremal Bell inequalities for $s_a = s_b = 2$ and three outcome measurements, and also $s_a = s_b = 3$ and two outcome measurements, without success. Note that states may have $(s, 1)$-extensions and no $(1, s)$-extensions, we have performed both tests in all cases. Although this possibility does not affect the overall conclusion, the states of [24] for example are sufficiently asymmetric with respect to swapping A and B that for $s = 2$ we found examples having one kind of extension but not the other, as well as states having both kinds (these are examples with (2, 2)-extensions which implies this latter condition).

We found that, although they have (2, 1)-extensions, only a few of the general complex UPB states of [27] have (3, 1)-extensions and similarly the C-H states have (3, 1)-extensions for a reduced range of values of $\alpha$. We did not find examples of Bruß-Peres states having (3, 1)-extensions.

Finally we considered Werner states [2] defined in dimensions $d = d_A = d_B \geq 2$ as $\rho_W = \frac{1}{d^2}(I(d - \Phi) + (d\Phi - 1)V)$ where $V$ is the flip operator. Werner [2] showed that for $\Phi \geq -1 + \frac{d^2}{d}$ these states do not violate any Bell inequality with an arbitrary number $s_a, s_b$ of von Neumann measurements (in Ref. [20] the author constructs LHV models for arbitrary POVM settings for a more restricted range of $\Phi$). We found that using symmetry techniques similar to those in Ref. [27] it is possible to analytically solve the dual optimization problem to the semi-definite program described above, see the Appendix. The value of the optimum establishes that all Werner states have symmetric extensions so long as $s_a + s_b \leq d$. Hence these states have LHV theories for all Bell experiments where the minimum number of settings $s = \min(s_a, s_b)$ satisfies $s + 1 \leq d$. This result is more general than Werner’s in the sense that, like in Ref. [20], it holds for general POVM elements. It is weaker in the sense that the number of settings is bounded by the dimension of the space. Numerical and analytical results (see Table II and the Appendix) show that Werner states for $d = 2$ actually have symmetric (quasi-)extensions beyond this analytically derived bound.

![Table II: Numerical results on the existence of symmetric extensions (ext) and decomposable quasi-extensions (q-ext) for $(s_a = 1, s_b = 2), (s_a = 2, s_b = 1), (s_a = 1, s_b = 3)$, and $(s_a = 3, s_b = 1)$.](image)

| C-H | Complex UPB | H-L | Bruß-Peres | Werner | Werner |
|-----|-------------|-----|------------|--------|--------|
| $\alpha \in [2, 4.33]$ | yes | yes | few | d ≥ 3 | $d \geq 4$ |
| $\alpha \in [2, 4.84]$ | yes | yes | few | $d \geq 3$ | $d \geq 4$ |
| $\alpha \in [2, 4.00]$ | yes | yes | few | $d \geq 3$ | $d \geq 4$ |

Even though our method is the most powerful tool to date for constructing local hidden variable theories, we believe that it is unlikely that every LHV model can be constructed from a symmetric quasi-extension. Our work is only the starting point for a more thorough exploration of the existence of (quasi-)extensions for entangled quantum states. In particular, it is an intriguing and open question whether there exist entangled states that have $(s_a = 1, s_b \to \infty)$ quasi-extensions. In fact we heard that it has been proved that only separable states have $(s_a = 1, s_b \to \infty)$ extensions [25, 26, 30].

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Appendix

In this Appendix we discuss the semidefinite program that constructs symmetric extensions in more detail and show that it is possible to construct symmetric extensions for many Werner states using our semi-definite programming approach. The ingredients of the argument are the semi-definite programming duality, the behavior of convex optimizations under symmetry and some simple group representation theory for the permutation group.

The semi-definite program that attempts to construct a symmetric extension has a natural dual that will turn out to be simpler to solve. We first review, for completeness, some standard descriptions and properties of semi-definite programs and their duals.

Vandenberghe and Boyd [18] write the general semidefinite program as

\[
\begin{align*}
& \text{minimize} & & c^T x, \\
& \text{subject to} & & F_0 + \sum_i x_i F_i \geq 0,
\end{align*}
\]

where \( c \) is a vector of length \( m \), and \((F_0, F_i)\) are \( n \times n \) Hermitian matrices with \( i = 1, \ldots, m \). The optimization variables form the vector \( x \), also of length \( m \). If there exists any vector \( x \) such that \( F(x) = F_0 + \sum_i x_i F_i > 0 \) the semi-definite program is said to be strictly feasible.

The dual optimization, also a semi-definite program, may be written

\[
\begin{align*}
& \text{maximize} & & -\text{Tr} F_0 Z, \\
& \text{subject to} & & Z \geq 0, \\
& & & \text{Tr} F_i Z = c_i,
\end{align*}
\]

where the optimization variable is the \( n \times n \) matrix \( Z \). Again, the dual semi-definite program is said to be strictly feasible if there is an \( Z > 0 \) satisfying the trace constraints.

The most important relation between the primal and dual optimizations is that \( \text{all allowed values of the primal objective function are greater than all allowed values of the dual objective function.} \) Thus feasible points of the dual problem can be used to bound the optimum of any semi-definite program. This property results from simply evaluating the difference between the primal and dual objective functions for any feasible pair \((x, Z)\)

\[
c^T x + \text{Tr} F_0 Z = \sum_i \text{Tr} x_i F_i Z + \text{Tr} F_0 Z = \text{Tr} F(x) Z \geq 0.
\]

The first equality results from the dual feasibility constraints and the inequality holds since \( \text{Tr} AB \) is positive if \( A \) and \( B \) are positive and Hermitian. Typically, the dual optimizations are more closely related, this is captured in Theorem 3.1 of [13]. If both the primal and dual forms of a semi-definite program are strictly feasible, their optimum are equal and achieved by some feasible pair \((x_{\text{opt}}, Z_{\text{opt}})\).

Comparing the semi-definite programs above with the semi-definite program for constructing symmetric extensions we see that it corresponds to the dual form defined above with \( F_i = \text{Sym}_A \otimes \text{Sym}_B(\sigma_i \otimes I) \), \( c_i = r_i = \text{Tr} \sigma_i \rho \) and \( F_0 = I_{d_A} \otimes I_{d_B} \otimes I \). We have \( m = (d_A d_B)^2 - 1 \) and \( n = d_A^2 d_B^2 \). The sign of the objective function was changed for clarity. Recall that there is a symmetric extension for \( \rho \) so long as the optimum is less than or equal to one. From now on we will write \( \text{Sym}' = \text{Sym}_A \otimes \text{Sym}_B \).

To see that this optimization is strictly feasible consider any, not necessarily positive, matrix \( K' \) satisfying the trace constraints \( (K')' \) exists since these constraints fix only a small number of the matrix elements of \( K' \). Then \( K = K' + \eta I_{d_A} \otimes I_{d_B} \otimes I \) is strictly positive so long as \( \eta > 0 \) is greater than the magnitude of the largest negative eigenvalue of \( K' \). \( K \) defined in this way still satisfies the trace constraints so the semi-definite program is strictly feasible. If we define the matrix \( X = I_{d_A} \otimes I_{d_B} + \sum x_i \sigma_i \), the dual form of our semi-definite program may be written

\[
\begin{align*}
& \text{maximize} & & 1 - \text{Tr} X \rho, \\
& \text{subject to} & & \text{Sym}'(X \otimes I) \geq 0.
\end{align*}
\]

The advantage of this semi-definite program from the point of view of analytical work is that the number of variables is very much smaller and we will see in the following that it can be further reduced by symmetry methods. Numerical implementations solve both optimizations at once. To see that this program is also strictly feasible consider the point \( x_i = 0 \) for all \( i \), for which \( X = I_{d_A} \otimes I_{d_B} \) and so \( \text{Sym}'(X \otimes I) \geq 0 \). From this we can conclude, by Theorem 3.1 of [13] as described above, that if the maximum of this optimization is less than or equal to one \( (\text{Tr} X_{\text{opt}} \rho \geq 0) \) there is a symmetric extension for \( \rho \). It is not necessary to construct the extension explicitly.

We now use the symmetry of the Werner states to simplify this semi-definite program. The Werner states have the property that \( (U \otimes U) \rho_W (U \otimes U)^\dagger = \rho_W \) for all unitary transformations \( U \) on \( \mathcal{H} [27] \). As a result the objective function is unchanged under the action \( X \rightarrow (U \otimes U) X (U \otimes U)^\dagger \) since \( \text{Tr} (U \otimes U) X (U \otimes U)^\dagger \rho_W = \text{Tr} X (U \otimes U)^\dagger \rho_W (U \otimes U) = \text{Tr} X \rho_W \). Similarly if we choose an \( X \) such that the positivity constraints are satisfied then

\[
U^\otimes(s_n + s_k) \text{Sym}'(X \otimes I) U^\dagger \otimes(s_n + s_k) \geq 0.
\]

On the other hand, \( U^\otimes(s_n + s_k) \) commutes with all matrices that permute the tensor factors and so it commutes with
the symmetrization operation. As a result
\[ \text{Sym}^{'((U \otimes U)X(U \otimes U)^\dagger \otimes I)} \geq 0. \]
So the set of allowed matrices \( X \) is also invariant under the operation \( X \to (U \otimes U)X(U \otimes U)^\dagger \). In fact since sums of positive matrices are positive convex combinations of matrices \((U \otimes U)X(U \otimes U)^\dagger\) for different \( U \) are also feasible and also achieve the same value of the objective function. As a result we may restrict our attention to matrices \( X \) such that \( \text{val}(U) \int (U \otimes U)X(U \otimes U)^\dagger dU = X \). For any feasible \( X \) of lower symmetry there is some feasible symmetrized matrix \( \hat{X} \) such that \( \text{Tr} \rho_W = \text{Tr} X \rho_W \). As discussed in [27] all the Hermitians matrices of this form may be written \( \hat{X} = x_1 I_{d_\lambda} \otimes I_{d_\mu} + xV \) for some real \( x_1 \) and \( x \). For the matrices \( X \) arising in our semi-definite program \( x_1 = 1 \) so we are left with a single variable optimization. (Note that there are general methods along these lines for reducing the dimensionality of semi-definite programs with symmetry [24, 23]. The key property is the convexity of the optimization.)

The objective function to be maximized for the Werner state is \( 1 - \text{Tr} X \rho_W = -x \Phi \). Since \( \rho_W \) is separable for \( \Phi \geq 0 \) we already know that an extension will exist for positive \( \Phi \) and can assume that \( \Phi \) is negative in the following. As a result we wish to find the maximum value of \( x \) for which the following matrix inequality holds
\[ f_d^{\otimes(s_a+s_b)} + x \text{Sym}^{'(V \otimes I)} \geq 0. \]

The eigenvalues of \( \text{Sym}^{'(X \otimes I)} \) are simply \( 1 + x \lambda_i \) where \( \lambda_i \) are the eigenvalues of \( \text{Sym}^{'(V \otimes I)} \). Supposing that the largest magnitude negative eigenvalue of \( \text{Sym}^{'(V \otimes I)} \) is \( -\lambda_m \), the optimum is \( x_{opt} = 1/\lambda_m \). Since the optimization is now over a single variable, the semi-definite program essentially reduces to an eigenvalue problem. The optimum of the semi-definite program will be \( -x_{opt} \Phi \) and if this is less than or equal to one there is a symmetric extension for \( \rho_W \). So \( \rho_W \) has a symmetric extension over the range \( -1/x_{opt} = -\lambda_m \leq \Phi \leq 1 \). Note that the symmetrization is a completely positive map and maps positive matrices \( X \) to positive matrices \( \text{Sym}^{'(X \otimes I)} \). Since \( X = I + xV \) is positive for \( -1 \leq x \leq 1 \), \( \text{Sym}^{'(X \otimes I)} \) must also be positive over this range so \( x_{opt} \geq 1 \).

To proceed further we must evaluate the smallest eigenvalue of \( \text{Sym}^{'(V \otimes I)} \). The matrix \( V \) swaps the Hilbert spaces belonging to Alice and Bob and therefore is an element of the representation of the group of permutations \( S_{s_a+s_b} \) that is made up of permutations of the \( s_a + s_b \) copies of \( H \). If \( \pi_{i,j} \) is the matrix that swaps the \( i \)-th and \( j \)-th spaces, we have \( V = \pi_{1,2} \). For clarity we will modify the order of the Hilbert spaces that we used above and imagine that odd-numbered spaces \( i = 1, 3, ..., s_a + s_b - 1 \) are copies of Alice’s system and that even-numbered spaces are copies of Bob’s.

As a preliminary, consider evaluating \( \text{Sym}(\sigma \otimes f_d^{\otimes(s-1)}) \) on \( H^{\otimes s} \). Clearly \( \sigma \otimes f_d^{\otimes(s-1)} \) is unaffected by any permutation that fixes the first object and so in some sense the only permutations that matter are the ones that swap the first Hilbert space with one of the others. More formally, we can divide the elements of the permutation group of \( s \) objects into cosets of the subgroup that fixes the first object. Any permutation can be realized by some permutation that fixes the first object followed by the transposition \( \pi_{1,i} \) for some \( i \) that labels which coset the permutation is in. Thus if we write the elements of the subgroup that fixes the first element as \( \tilde{\pi} \) we have
\[ \text{Sym}(H) = \frac{1}{s!} \sum_{\pi} \pi_H \pi^\dagger \]
\[ = \frac{1}{s!} \sum_{\pi} \pi_{1,i} \left( \frac{1}{(s-1)!} \sum_{\pi} \pi_H \pi^\dagger \right) \pi_{1,i}. \]

Finally, \( \sigma \otimes I_d^{\otimes(s-1)} \) maps to itself under all \( \pi \) so \( \text{Sym}(\sigma \otimes f_d^{\otimes(s-1)}) = \sum_{\pi} \pi_{1,i} \) gives
\[ \text{Sym}^{'(V \otimes I)} = \frac{1}{s_a s_b} \sum_{i=1}^{s_a} \sum_{j=1}^{s_b} \pi_{2(i-1,2j)}. \]

So the symmetrized matrix reduces to a linear combination of transpositions of Hilbert spaces.

The matrices \( \pi \) form a reducible unitary representation of the symmetric group \( S_{s_a+s_b} \). There is a single unitary transformation that will block-diagonalize all the \( \pi \) with the blocks being, possibly repeated, irreducible representations of the group (see for example [31]). Since this is a single unitary transformation applied to all \( \pi \) it does not change the eigenvalues of linear combinations of different \( \pi \). Such linear combinations will be positive if and only if all the blocks are positive and so we can restrict our attention to the eigenvalues of the blocks of \( \text{Sym}^{'(V \otimes I)} \) in this basis. Now suppose that the alternating representation occurs in this decomposition at least once. Since in this irreducible representation even permutations are represented by 1 and odd ones by \(-1\), the value of this block of \( \text{Sym}^{'(V \otimes I)} \) is \(-1\). This implies that \( x_{opt} \leq 1 \). Combined with the earlier lower bound on the optimum we have \( x_{opt} = 1 \) and \( \rho_W \) has a symmetric extension for all allowed values \(-1 \leq \Phi \leq 1 \).

It is a standard result that the alternating representation occurs in the decomposition into irreducibles of the representation of \( S_{s_a+s_b} \) by permutations of tensor factors of \( H_d^{\otimes(s_a+s_b)} \) so long as \( s_a + s_b \leq d \) [44]. In fact it is easy to see that the alternating representation occurs if and only if there is a non-trivial completely antisymmetric subspace of \( H_d^{\otimes(s_a+s_b)} \). This completes the argument. All Werner states have a \((s_a,s_b)\)-symmetric extension and an LHV theory for all Bell experiments with \((s_a,s_b)\) settings if \( s_a + s_b \leq d \).
Note that the converse is not true, a symmetric extension may exist even if this condition is not met. Consider $s_a = s_b = 2$ and $d = 2$. In both these cases the decomposition includes the two-dimensional irreducible representation of $S_4$ [1] that can be generated by

$$\tilde{\pi}_{(1,2)} = \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix} = \tilde{\pi}_{(3,4)}, \quad \tilde{\pi}_{(2,3)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$  

Any block corresponding to this irrep is then equal to

$$\left(\tilde{\pi}_{(1,2)} + \tilde{\pi}_{(1,4)} + \tilde{\pi}_{(2,3)} + \tilde{\pi}_{(3,4)}\right)/4 = \begin{pmatrix} 0 & -\frac{1}{2} \\ -\frac{1}{2} & 0 \end{pmatrix}.$$  

Since this has eigenvalues $(-1/2, 1/2)$ we have $x_{opt} \leq 2$. It is straightforward to check the blocks corresponding to the other irreducible representations to confirm that $x_{opt} = 2$. As a result we may say that Werner states in two dimensions have $(2,2)$, $(2,1)$ and $(1,2)$-extensions if $-1/2 \leq \Phi \leq 1$. It is straightforward to confirm numerically that the same statement applies to decomposable $(2,2)$-quasi-extensions. The irreducible representations of $S_n$ for large $n$ are typically high dimensional. Note, however, that further block diagonalization is possible in principle since $\text{Sym}^2(V \otimes I)$ is invariant under any permutation of Alice’s spaces or of Bob’s. This means that each block of $\text{Sym}^2(V \otimes I)$ is in the commutant algebra of the reducible representation of $S_n \times S_n$, that arises from restricting an irreducible representation of $S_n \times S_n$ to a representation of $S_{n_a} \times S_{n_b}$. This commutant algebra will typically have very much smaller block size.

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[32] In the literature one encounters both a weak as well as a strong version of a local hidden variable test. In the weak version the goal is to reproduce the expectation value of a set of local observables on a particular quantum system by means of a local hidden variable model. In the strong version one attempts to reproduce the exact probabilities of outcome for a set of local measurements by means of a local hidden variable model. All the results in this paper hold for the stronger model.

[33] A connection between Bell inequalities and extensions has been made previously by R.F. Werner [17] who used violations of a CHSH inequality to show that there exist quantum states on AB and A’B with a common reduction on B for which there is no joint quantum state on AA’B. In the case where the states on AB and A’B are required to be the same, the existence of such a joint state implies the existence of a symmetric extension.