The quantum moment problem
and bounds on entangled multi-prover games

Andrew C. Doherty∗  Yeong-Cherng Liang∗  Ben Toner†  Stephanie Wehner‡

March 31, 2008

Abstract

We study the quantum moment problem: Given a conditional probability distribution together with some polynomial constraints, does there exist a quantum state $\rho$ and a collection of measurement operators such that (i) the probability of obtaining a particular outcome when a particular measurement is performed on $\rho$ is specified by the conditional probability distribution, and (ii) the measurement operators satisfy the constraints. For example, the constraints might specify that some measurement operators must commute.

We show that if an instance of the quantum moment problem is unsatisfiable, then there exists a certificate of a particular form proving this. Our proof is based on a recent result in algebraic geometry, the noncommutative Positivstellensatz of Helton and McCullough [Trans. Amer. Math. Soc., 356(9):3721, 2004].

A special case of the quantum moment problem is to compute the value of one-round multi-prover games with entangled provers. Under the conjecture that the provers need only share states in finite-dimensional Hilbert spaces, we prove that a hierarchy of semidefinite programs similar to the one given by Navascués, Pironio and Acín [Phys. Rev. Lett., 98:010401, 2007] converges to the entangled value of the game. It follows that the class of languages recognized by a multi-prover interactive proof system where the provers share entanglement is recursive.

∗School of Physical Sciences, The University of Queensland, Queensland 4072, Australia
†Centrum voor Wiskunde en Informatica, Kruislaan 413, 1098 SJ Amsterdam, The Netherlands
‡Institute for Quantum Information, California Institute of Technology, Pasadena, CA 91125, USA
1 Introduction

The study of multi-prover games has led to many exciting results in classical complexity theory. A one-round multi-prover cooperative game of incomplete information is a game played by a verifier against two provers, Alice and Bob. The strategy of the verifier is fixed. He randomly chooses two questions according to some fixed probability distribution and sends one question to each prover. Alice and Bob then each return an answer to the verifier. The verifier decides whether to accept these answers on the basis of some pre-defined rules of the game that specify whether the given answers are winning answers for the questions sent. To win the game, Alice and Bob may thereby agree on any strategy beforehand, but they may no longer communicate once the game has started. The maximum probability with which Alice and Bob can cause the verifier to accept is known as the value of the game. A simple example is the well-known CHSH game \[14, 15\]. In this case, the questions and answers are bits. The verifier chooses questions \(s \in \{0, 1\}\) and \(t \in \{0, 1\}\) uniformly at random and sends \(s\) to Alice and \(t\) to Bob. In order to win the game, Alice and Bob must reply with bits \(a, b \in \{0, 1\}\) such that \(s \land t = a \oplus b\), i.e., the logical AND of \(s\) and \(t\) should be equal to the XOR of \(a\) and \(b\). It is straightforward to verify that the CHSH game has value \(3/4\).

Interactive proof systems have received considerable attention since their introduction by Babai \[2\] and Goldwasser, Micali and Rackoff \[20\] in 1985. Of special interest to us are proof systems with multiple provers \[3, 5, 10, 17, 18, 29\] as introduced by Ben-Or, Goldwasser, Kilian and Widgerson \[5\], which can be described in terms of multi-prover games between a verifier, and two or more provers. Whereas the provers are computationally unbounded, the verifier is limited to probabilistic polynomial time. Both the provers and the verifier have access to a common input string \(x\). The goal of the provers is to convince the verifier that \(x\) belongs to a pre-specified language \(L\). The verifier’s aim, on the other hand, is to determine whether the provers’ claim is indeed valid. In each round, the verifier sends a \(\text{poly}(|x|)\) size query to the provers, who return a polynomial size answer. At the end of the protocol, the verifier either accepts, meaning that he concludes \(x \in L\), or rejects, based on the messages exchanged and his own private randomness. A language \(L\) has a multi-prover interactive proof system if there is a protocol such that, if \(x \in L\), there exist answers the provers can give which will cause the verifier to accept with high probability. However, if \(x \notin L\), then there exists no strategy for the provers that will only cause the verifier to accept, except with very low probability. Here, \(x\) and \(L\) lead to particular game. Let \(\text{MIP}\) denote the class of languages having a multi-prover interactive proof system. It has been shown that classical two-prover interactive proof systems are just as powerful as proof systems involving more than two provers. Indeed, Babai, Fortnow and Lund \[3\], and Feige and Lovász \[18\] have shown that a language is in \(\text{NEXP}\) if and only if it has a two-prover one-round proof system, i.e., \(\text{MIP} = \text{NEXP}\).

1.1 Multi-prover games with entanglement

In this paper, we study multi-prover games in a quantum setting. In particular, we allow Alice and Bob to share an entangled quantum state as part of their strategy. After receiving their questions, the provers may perform any local measurement on their part of the entangled state, and decide on an answer based on the outcome of their measurement. All communication between the verifier and the provers remains classical. It turns out that sharing entanglement can increase the probability that the provers can cause the verifier to accept, an effect known as quantum nonlocality. For example, if the provers share a maximally entangled state of two qubits they can win the CHSH game (cause the verifier to accept) with probability \(p_{\text{CHSH}} \approx 85% > 3/4\).
We write $\text{MIP}^*$ for the set of languages that have interactive proofs with entangled provers. Very little is known about $\text{MIP}^*$. Most importantly, it was not known before our work whether there exists an algorithm of any complexity for deciding membership in $\text{MIP}^*$, except for extremely restricted classes of games. In particular, if we restrict to games where Alice and Bob each answer a single bit $a, b \in \{0, 1\}$, and the verifier only looks at the XOR of these two bits, then the (entangled) value of the game can be computed in time polynomial in the number of questions [12, 15]. Let $\oplus \text{MIP}[2]$ denote the restricted class where the verifier’s output is a function of the XOR of two binary answers. Then $\oplus \text{MIP}^*[2] \subseteq \text{EXP}$ [13], while it is known that $\oplus \text{MIP} = \text{NEXP}$, for certain completeness and soundness parameters [22], i.e., the resulting proof system is significantly weakened if the provers are allowed to share entanglement. In fact, such a proof system can even be simulated using just a single quantum prover, i.e., $\oplus \text{MIP}^*[2] \subseteq \text{QIP}(2) \subseteq \text{EXP}$ [18, 27].

Unfortunately, very little is known for more general games where we allow shared entanglement between the provers, and where Alice and Bob give much longer answers, or when we have more than two provers. Unlike in the classical case, general multi-prover games are not equivalent to two-prover games when the provers share entanglement [25]. For two-prover unique games (where for each pair of questions there exists exactly one pair of winning answers), it is known that we can approximate the value of a two-prover game to within a certain accuracy in polynomial time [26]. Masanes [33] has shown how to compute the value of multi-prover games where the questions to, and the answers from each prover are bits. But even for very small games with a very limited number of questions, the entangled value is typically unknown [9].

Assuming that the provers share quantum entanglement is a reasonable model because it captures the properties of a multi-prover game that a verifier can enforce physically: while the verifier can enforce the condition that the provers cannot communicate by ensuring that they are spacelike-separated, he has no way to ensure that provers in a quantum universe do not share entanglement. Multi-prover games with entangled provers are also known as non-local games with entanglement. The entangled value of a game is the maximum probability with which Alice and Bob can win using entanglement. Here, we are concerned with the following question: How can we compute the entangled value of non-local games with multiple provers? And, how can we decide membership of $\text{MIP}^*$?

1.2 Results

Quantum moment problem. To reach our goal, we first introduce the quantum moment problem that is a generalization of our problem. Informally, the quantum moment problems asks whether given a conditional probability distributions and some polynomial constraints on observables, we can find a quantum state and quantum measurements satisfying the constraints, that provide us with the required probabilities. We may use the constraints to impose certain restrictions on the form of our quantum measurements. For example, we may want to demand that two measurement operators act on two or more distant subsystems independently. Determining whether there is an entangled strategy for a multi-prover game that achieves a certain winning probability is a special case of the quantum moment problem.

Other special cases of the quantum moment problem include the so-called classical marginal problem [31], which asks whether given certain marginal distributions, we can find a joint distribution that has the desired marginals. Our problem is also closely related to the quantum marginal problem in which the aim is to find a density matrix for a multipartite quantum system that is consistent with a specified set of reduced density matrices for specific subsystems. This problem is
QMA-complete and has attracted a lot of interest recently [32]. A special case is \( N \)-representability, an important problem with a long history in quantum chemistry [28]. One key difference between our quantum moment problem and the quantum marginal problem is that in the latter case the dimension of the quantum state, and its various subsystems, is specified. In the quantum moment problem the aim is to find a state satisfying the given constraints in a quantum system of any, possibly infinite, dimension. Finally, it may also be possible to treat games with quantum verifier within the framework of the quantum moment problem.

**Refuting unsatisfiable instances.** We describe a general way of proving that an instance of a quantum moment problem is unsatisfiable. The proof follows from a recent result of Helton and McCullough [23], a Positivstellensatz for polynomials in noncommuting variables. The choice of polynomials will define a particular instance of the quantum moment problem, where the variables correspond to measurement operators. In Helton and McCullough’s result the noncommuting variables are required to satisfy certain polynomial equality and inequality constraints but can be evaluated in any quantum system, even one of infinite dimensions. Informally, the Positivstellensatz states that any such polynomial that is positive can be written a sum of squares, a form that makes it obvious that the polynomial is positive. By positive we mean that, whenever the constraints are satisfied, the polynomial is positive semidefinite, i.e. it has a positive expectation value for all quantum states in whatever quantum system. Such a representation as a sum of squares acts as a certificate for the unsatisfiability of an instance of a quantum moment problem. Certificates of this kind have often been used in the theoretical physics literature to place very general bounds on quantum correlations (see for example [19]). Helton and McCullough’s result shows that such certificates are all that is ever required to demonstrate that an instance of the quantum moment problem is unsatisfiable.

**Tensor products and commutation.** In order to apply the Positivstellensatz to obtain bounds on the entangled values of two-prover games, we need to incorporate a constraint in the corresponding quantum moment problem that ensures Alice and Bob’s measurements act on different subsystems \( \mathcal{H}_A \) and \( \mathcal{H}_B \). When Alice and Bob share a quantum system of some finite dimension, this means that one demands that the Hilbert space \( \mathcal{H} \) describing this system decomposes as \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). Alice and Bob’s measurements should be of the form \( A_s \otimes B_t \) with \( A_s \in \mathcal{H}_A \) and \( B_t \in \mathcal{H}_B \) for all questions \( s \) and \( t \). Unfortunately, we can only apply the Positivstellensatz when the constraints are polynomials in \( A_s \) and \( B_t \). Thus we need an additional trick to impose an explicit tensor product structure. To get around this problem, we demand that for all \( s \) and \( t \) we have \( [A_s, B_t] = 0 \), i.e., that all measurement operators of Alice commute with all those of Bob. If the Hilbert space is finite-dimensional, then imposing the commutativity constraints is actually equivalent to demanding a tensor product structure. This result is well-known in the mathematical physics literature [45]. Here, we provide a simple version of this argument accessible from a computer science perspective, which directly applies to our analysis of multi-prover games.

From a physics point of view, however, the usual requirement on observables that can be measured in space-like separated regions is that they should commute, not that they should have a tensor product factorization. Indeed, this commutativity requirement on local observables is regarded by many as an axiom that should be satisfied by any reasonable quantum mechanical theory of nature [21]. Unfortunately, when the algebra of observables cannot be represented on a finite-dimensional Hilbert space it is an open question whether this commutativity property
implies the existence of a tensor product factorization. Our results will provide bounds on the values of multi-prover games that are valid for all quantum systems whenever the observables of different players commute. We will refer to the maximum probability of winning a game \( G \) with (possibly) infinite-dimensional operators satisfying commutativity constraints as the field-theoretic value \( \omega_f(G) \) of the game. It is an open question whether this is the same as the usual entangled value of the game. Since MIP\(^*\) was defined with a tensor product structure in mind, we here define the class MIP\(^f\), where the tensor products are replaced by the commutative requirement. The class MIP\(^f\) seems more appropriate to our main motivation of studying the power of multi-prover games where the provers are only limited by what they can achieve physically. Restricting Alice and Bob to sharing finite-dimensional systems does not seem natural from a physical perspective.

A hierarchy of semidefinite programs. We know that the Positivstellensatz leads to certificates that tell us when a particular quantum moment problem is unsatisfiable. But how can we find such certificates? If we place a bound on the size of the certificate, then the problem of determining whether there exists a certificate of that size can be formulated as a semidefinite program (SDP) [47, 6]. In particular, searching for certificates of increasing size yields a hierarchy of SDPs. The resulting hierarchy is very similar to the one presented in a groundbreaking paper of Navascu´es, Pironio and Ac´ın [36], which partly motivated this work.

In many applications, including multi-prover games, we are not only interested in whether a specific instance of the moment problem is satisfiable but in finding the best possible bound on some linear combination of moments. Once again fixing the size of the certificates of infeasibility straightforwardly leads to a hierarchy of SDPs that provide progressively tighter bounds. For multi-prover games \( G \), it was previously not known whether the solutions to this hierarchy of SDPs converged to the entangled value of the game, which we denote by \( \omega^*(G) \). Here we almost show this. What we actually show is that the hierarchy converges to the field-theoretic value (see above) of a non-local game \( G \). In the language of the quantum moment problem, we wish to know if there exists an entangled strategy for \( G \) such that the provers win with some fixed probability \( p \). However, the Positivstellensatz only yields a certificate that there is no entangled strategy that wins with probability \( p \) if there is also no such strategy even with infinite-dimensional measurement operators. If the measurement operators are infinite-dimensional, then the commutativity constraints do not necessarily imply the existence of a tensor product structure. In other words, we show that our hierarchy converges to the field-theoretic value of the game.

MIP\(^*\) is recursive. Since our hierarchy converges, we can compute the value of an entangled game and hence obtain an algorithm for deciding membership of MIP\(^*\) (under the assumption that the optimal value is achieved with finite-dimensional operators) and of MIP\(^f\). This implies that these classes are recursive.

Examples: The \( I_{3322} \) inequality and Yao’s inequality. Finally, we demonstrate the power of our technique by providing an extremely simple, algorithmically constructed, certificate bounding the value of a two-party Bell inequality [4] known as the \( I_{3322} \) inequality [16], and a multi-player non-local game suggested by Yao and collaborators [50].
1.3 Open Questions

With respect to the above discussion, it would be interesting to know whether there are games \( G \) such that \( \omega^*(G) \) is strictly less than \( \omega^f(G) \). Can it really help the provers to have infinite-dimensional systems when the number of questions and answers in the game are finite? One way to establish that there is no advantage to having infinite-dimensional systems would be to ‘round’ the SDP hierarchy directly to a quantum strategy with finite entanglement, bypassing the (nonconstructive) Positivstellensatz altogether. For XOR-games, the first level of our hierarchy is tight and it is well-known how a solution of the SDP can be transformed into a quantum strategy via so-called Tsirelson’s vector construction \[11, 12, 13\]. However, there exist many non-local games, for which the first level of the hierarchy does not provide us with the optimal value of the game, but merely gives us an upper bound. This fact alone shows that for general games, we cannot find such a nice embedding of vectors into observables as can be done for XOR-games. However, something similar may still be possible for restricted classes of games, exhibiting a likewise special structure.

We also do not establish anything about the rate of convergence of the SDP hierarchy. In some numerical experiments with small games, the low levels of the SDP hierarchy do yield optimal solutions. Establishing this in general would provide an upper bound on \( \text{MIP}^* \). We have made partial progress on this question by proving convergence for a particular hierarchy of SDPs.

1.4 Related work

In Ref. \[36\], a paper which partly inspired this work, Navascués, Pironio, and Acín (NPA), defined a closely related semidefinite programming hierarchy. Subsequently, and independently of us, NPA have proved that their semidefinite programming hierarchy converges to the field-theoretic value of the game \[34\]. Our paper and theirs are complementary: While our work emphasizes the connection with Positivstellensatz of Helton and McCullough, NPA prove convergence directly. Their proof has a number of advantages: most notably, when their hierarchy converges to the field-theoretic value of the game at a finite level, NPA obtain a bound on the dimension of the state required to reproduce the correlations. NPA have also shown that their new technique for proving convergence can be extended to general polynomial optimization problems in noncommutative variables \[35\].

Finally, our techniques have recently extended by Ito, Hirotada, and Matsumoto to the case of games with quantum messages between verifier and provers \[24\].

1.5 Outline

In Section 2 we provide an introduction to non-local games including all necessary definitions. Section 3 then defines the quantum moment problem, and Section 4 introduces our main tools. In particular, Section 4.1 provides an explanation of why we obtain a tensor product structure from commutation relations, and in Section 4.2 we show that if a quantum moment problem is unsatisfiable, we can find certificates of this fact using the Positivstellensatz. We then use these tools in our SDP hierarchy in Section 5 and conclude in Section 5.2 with some explicit examples.
2 Preliminaries

2.1 Notation

We assume general familiarity with the quantum model \[37\]. In the following, we use \( A^\dagger \) to denote the conjugate transpose of a matrix \( A \). A matrix is Hermitian if and only if \( A^\dagger = A \). We write \( A \geq 0 \) to indicate that a matrix \( A \) is positive semidefinite, i.e., it is Hermitian and has no negative eigenvalues. We also use \( A = 0 \) to express that \( A \) is the all-zero matrix and \( A \neq 0 \) to indicate that \( A \) has at least one non-zero entry. The \((i,j)\)-entry of \( A \) will be denoted by \([A]_{i,j}\). For two matrices \( A \) and \( B \) we write their commutator as \([A, B] = AB - BA\). We use \( \mathbb{H} \) to denote a Hilbert space and \( \mathcal{H}_k \) the Hilbert space belonging to subsystem \( k \). \( I_k \) is the identity on system \( k \), and \( \mathbb{B}(\mathcal{H}) \) denotes the set of all bounded operators on the Hilbert space \( \mathcal{H} \). Unless stated otherwise, we take all systems to be finite-dimensional. We will also employ the shorthand \( \mathbb{B}(\mathcal{H}) \times_n := \mathbb{B}(\mathcal{H}) \times \ldots \times \mathbb{B}(\mathcal{H}) \) for the \( n \)-fold Cartesian product of \( \mathbb{B}(\mathcal{H}) \), and let \( |n| := \{1, \ldots, n\} \). Furthermore, we will use \(|S|\) and \(|L|\) to denote the number of elements of a set \( S \) and list \( L \) respectively.

For the purpose of subsequent discussion, we now note that a Hermitian polynomial \( p(X) \) in noncommutative variables \( X = (X_1, \ldots, X_k) \) is a sum of squares (SOS) if there exist polynomials (matrices) \( r_j \) of appropriate dimension such that
\[
p(X) = \sum_j r_j^\dagger r_j.
\]

It is important to note that if \( p(X) \) is an SOS polynomial, it is also a positive semidefinite matrix, i.e., \( p(X) \geq 0 \).

2.2 Games

As an example application of the quantum moment problem, we will consider cooperative games among \( n \) parties. For simplicity, we first describe the setting for only two parties, henceforth called Alice and Bob. A generalization is straightforward. Let \( S, T, A \) and \( B \) be finite sets, and \( \pi \) a probability distribution on \( S \times T \). Let \( V \) be a predicate on \( S \times T \times A \times B \). Then \( G = G(V, \pi) \) is the following two-person cooperative game: A pair of questions \((s, t) \in S \times T\) is chosen at random according to the probability distribution \( \pi \). Then \( s \) is sent to Alice, and \( t \) to Bob. Upon receiving \( s \), Alice has to reply with an answer \( a \in A \). Likewise, Bob has to reply to question \( t \) with an answer \( b \in B \). They win if \( V(s, t, a, b) = 1 \) and lose otherwise. Alice and Bob may agree on any kind of strategy beforehand, but they are no longer allowed to communicate once they have received questions \( s \) and \( t \). The value \( \omega(G) \) of a game \( G \) is the maximum probability that Alice and Bob win the game. In what follows, we will write \( V(a, b|s, t) \) instead of \( V(s, t, a, b) \) to emphasize the fact that \( a \) and \( b \) are answers given questions \( s \) and \( t \).

Here, we are particularly interested in non-local games and where Alice and Bob are allowed to share an arbitrary entangled state \(|\psi\rangle\) to help them win the game. Let \( \mathcal{H}_A \) and \( \mathcal{H}_B \) denote the Hilbert spaces of Alice and Bob respectively. The state \(|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B \) is part of the quantum strategy that Alice and Bob can agree on beforehand. This means that for each game, Alice and Bob can choose a specific \(|\psi\rangle \) to maximize their chance of success. In addition, Alice and Bob can
agree on quantum measurements where we may without loss of generality assume that these are projective measurements \[15\]. For each \(s \in S\), Alice has a projective measurement described by \(\{ A^a_s : a \in A\} \) on \(\mathcal{H}_A\). For each \(t \in T\), Bob has a projective measurement described by \(\{ B^b_t : b \in B\} \) on \(\mathcal{H}_B\). For questions \((s, t) \in S \times T\), Alice performs the measurement corresponding to \(s\) on her part of \(| \psi \rangle\) which gives her outcome \(a\). Likewise, Bob performs the measurement corresponding to \(t\) on his part of \(| \psi \rangle\) with outcome \(b\). Both send their outcome, \(a\) and \(b\), back to the verifier. The probability that Alice and Bob answer \((a, b) \in A \times B\) is then given by

\[
\langle \psi | A^a_s \otimes B^b_t | \psi \rangle.
\]

We can now define:

**Definition 2.1.** The *entangled value* of a two-prover game with classical verifier \(G = G(\pi, V)\) is given by:

\[
\omega^*(G) = \lim_{d \to \infty} \max_{\| \psi \| = 1} \max_{\pi \in C^d \otimes C^d} \sum_{a, b, s, t} \pi(s, t)V(a, b|s, t)\langle \psi | A^a_s \otimes B^b_t | \psi \rangle,
\]

where \(A^a_s \in \mathbb{B}(\mathcal{H}_A)\) and \(B^b_t \in \mathbb{B}(\mathcal{H}_B)\) for some Hilbert space \(\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B\), satisfying \(A^a_s, B^b_t \geq 0\), \(\sum_a A^a_s = \mathbb{I}_A\), \(\sum_b B^b_t = \mathbb{I}_B\) for all \(s \in S\) and \(t \in T\).

We also define a more general version of this statement, which will provide an upper bound to the quantum value of the game:

**Definition 2.2.** The *field-theoretic value* of a two-prover game with classical verifier \(G = G(\pi, V)\) is given by:

\[
\omega^f(G) = \sup_{A^a_s, B^b_t} \left\| \sum_{a, b, s, t} \pi(s, t)V(a, b|s, t)A^a_s B^b_t \right\|,
\]

where \(\|O\|\) is the operator norm of \(O\), \(A^a_s \in \mathbb{B}(\mathcal{H}_A)\) and \(B^b_t \in \mathbb{B}(\mathcal{H}_B)\) for some Hilbert space \(\mathcal{H}\), satisfying \(A^a_s, B^b_t \geq 0\), \(\sum_a A^a_s = \sum_b B^b_t = \mathbb{I}\) for all \(s, t\), and \([A^a_s, B^b_t] = 0\) for all \(s \in S\), \(t \in T\), \(a \in A\), and \(b \in B\).

**Lemma 2.3.** Let \(G = G(\pi, V)\) be a two-prover game with classical verifier. Then \(\omega^*(G) \leq \omega^f(G)\).

**Proof.** Let \(\varepsilon > 0\). Choose \(d\) sufficiently large so that there is a normalized state \(| \psi \rangle\) and operators \(A^a_s, B^b_t\) defining a strategy with winning probability at least \(\omega^*(G) - \varepsilon\). Let \(\tilde{A}^a_s = A^a_s \otimes \mathbb{I}_B\) and \(\tilde{B}^b_t = \mathbb{I}_A \otimes B^b_t\). Then \(\tilde{A}^a_s\) and \(\tilde{B}^b_t\) are positive semidefinite operators on \(\mathbb{C}^{d^2}\) satisfying all the conditions in Definition 2.2. Finally,

\[
\omega^f(G) = \sup_{\tilde{A}^a_s, \tilde{B}^b_t} \left\| \sum_{a, b, s, t} \pi(s, t)V(a, b|s, t)\tilde{A}^a_s \tilde{B}^b_t \right\|
\]

\[
\geq \left\| \sum_{a, b, s, t} \pi(s, t)V(a, b|s, t)\tilde{A}^a_s \tilde{B}^b_t \right\|
\]

\[
\geq \langle \psi | \left( \sum_{a, b, s, t} \pi(s, t)V(a, b|s, t)\tilde{A}^a_s \tilde{B}^b_t \right) | \psi \rangle
\]

\[
\geq \omega^*(G) - \varepsilon.
\]

\(^1\)By Neumark’s theorem, any generalized measurements described by positive-operator-valued measure can be implemented as projective measurements in some higher dimensional Hilbert space. See, for example, pp. 285 of Ref. [10].
Since $\varepsilon$ was arbitrary, the result follows. \hfill \square

In our examples, we will sometimes use the term *Bell inequality* [4] to refer to a particular non-local game. This is an equivalent formulation, where we only consider terms of the form $\langle \psi | A_s^a B^b_t | \psi \rangle$. The value of the game can then be obtained by averaging. In inequalities where Alice and Bob have, respectively, two measurement outcomes for each possible choice of measurement setting (i.e., $A = B = \{0, 1\}$), their measurements can be described by observables of the form $A_s = A^0_s - A^1_s$ and $B_t = B^0_t - B^1_t$ respectively. In this case, we state inequalities in the form of the observables $A_s$ and $B_t$ where we will use the shorthand $\langle A_s B_t | \psi \rangle$.

Note that it is straightforward to extend the above definitions to the setting involving multiple players, but the resulting terms will be much harder to read. When considering games among $N$ players $P_1, \ldots, P_N$, let $S_1, \ldots, S_N$ and $A_1, \ldots, A_N$ be finite sets corresponding to the possible questions and answers respectively. Let $\pi$ be a probability distribution on $S_1 \times \ldots \times S_N$, and let $V$ be a predicate on $A_1 \times \ldots \times A_N \times S_1 \times \ldots \times S_N$. Then $G = G(V, \pi)$ is the following $N$-player cooperative game: A set of questions $(s_1, \ldots, s_N) \in S_1 \times \ldots \times S_N$ is chosen at random according to the probability distribution $\pi$. Player $P_j$ receives question $s_j$, and then responds with an answer $a_j \in A_j$. The players win if and only if $V(a_1, \ldots, a_N|s_1, \ldots, s_N) = 1$. Let $|\psi\rangle$ denote the players’ choice of state, and let $X_j := \{ |a_j\rangle \, | a_j \in A_j \}$ denote the positive-operator-valued measurement (POVM) of player $P_j$ for question $s_j \in S_j$, i.e., $\sum_{a_j} X_{s_j}^{a} = I$ and $X_{s_j}^{a} \geq 0$ for all $a_j$. The value of the game can now be written as

$$
\omega^*(G) = \lim_{d \to \infty} \max_{\omega \in (C^d)^\otimes N} \max_{X_1, \ldots, X_N} \sum_{s_1, \ldots, s_N} \pi(s_1, \ldots, s_N) \sum_{a_1, \ldots, a_N} V(a_1, \ldots, a_N|s_1, \ldots, s_N) \langle \psi | X_{s_1}^{a_1} \otimes \ldots \otimes X_{s_N}^{a_N} | \psi \rangle,
$$

where the maximization is taken over all legitimate POVMs $X_j$ for all $j \in [N]$. Similarly, we can now write the field-theoretic value of the game as

$$
\omega^f(G) = \sup_{X_1, \ldots, X_N} \left\| \sum_{s_1, \ldots, s_N} \pi(s_1, \ldots, s_N) \sum_{a_1, \ldots, a_N} V(a_1, \ldots, a_N|s_1, \ldots, s_N) X_{s_1}^{a_1} \ldots X_{s_N}^{a_N} \right\|,
$$

where we now have $\sum_{a_j} X_{s_j}^{a_j} = I$ for all $a_j, s_j, j$ and $[X_{s_j}^{a_j}, X_{s_j}^{a'_{j'}}] = 0$ for all $j \neq j'$.

### 2.3 Proof systems

Interactive proof systems can be phrased as such games. For completeness, we here provide a definition of MIP. We refer to the introduction and the previous section for an explanation of the notions of a tensor product form vs. commutation relations.

**Definition 2.4.** For $0 \leq s < c \leq 1$, let $\oplus\text{MIP}^{s,c}[k]$ denote the class of all languages $L$ recognized by a classical $k$-prover interactive proof system with entanglement such that:

- The interaction between the verifier and the provers is limited to one round and classical communication. The verifier chooses $k$ questions from a finite set of possible questions, according to a fixed probability distribution known to the provers, and sends one question to each prover. Afterwards, the provers may perform any measurement that has tensor product form on a shared state $|\psi\rangle$ that they have chosen ahead of time. Each prover returns an answer to the verifier, whose decision function is known to the provers.

8
• If $x \in L$ then there exists a strategy for the provers for which the probability that the verifier accepts is at least $c$ (the completeness parameter).

• If $x \notin L$ then, whatever strategy the $k$ provers follow, the probability that the verifier accepts is at most $s$ (the soundness parameter).

Definition 2.5. For $0 \leq s < c \leq 1$, let $\oplus \text{MIP}^f_{c,s}[k]$ denote the class corresponding to a modified version of the previous definition: here we merely ask that the measurements operators between the different players commute.

3 The quantum moment problem

3.1 General form

Let us now state the quantum moment problem in its most general form, before explaining its connection to non-local games. Intuitively, the quantum moment problem states that given a certain probability distribution, is it possible to find quantum measurements and a state that provide us with such a distribution?

Definition 3.1 (Quantum moment problem). Given a list of numbers $\mathcal{M} = (m_i \mid m_i \in [0, 1])$, a set of polynomial equations $\mathcal{R} = \{r = 0 \mid r : \mathbb{B}(\mathcal{H})^{\times |\mathcal{M}|} \rightarrow \mathbb{B}(\mathcal{H})\}$, and polynomial inequalities $\mathcal{S} = \{s \geq 0 \mid s : \mathbb{B}(\mathcal{H})^{\times |\mathcal{M}|} \rightarrow \mathbb{B}(\mathcal{H})\}$, does there exist said Hilbert space $\mathcal{H}$, operators $M_i \in \mathbb{B}(\mathcal{H})$ and a state $\rho \in \mathbb{B}(\mathcal{H})$ such that

1. For all $m_i \in \mathcal{M}$, $\text{Tr}(M_i \rho) = m_i$.

2. For all $r \in \mathcal{R}$, $r(M_1, \ldots, M_{|\mathcal{M}|}) = 0$.

3. For all $s \in \mathcal{S}$, $s(M_1, \ldots, M_{|\mathcal{M}|}) \geq 0$.

3.2 Non-local games

In this paper, we are particularly interested in a special case of the quantum moment problem, where we consider measurements on many space-like separated systems as in the setting of non-local games. For simplicity, we will explain the connection to non-local games for only two such systems, Alice $\mathcal{H}_A$ and Bob $\mathcal{H}_B$, where it is straightforward to extend our arguments to more than two. On each system $\mathcal{H}_A$ and $\mathcal{H}_B$, we want to perform a finite set of possible measurements $S$ and $T$ each of which has the same finite set of outcomes $A$ and $B$ respectively. Let $m^A(a|s)$ and $m^B(b|t)$ denote the probability that on systems $\mathcal{H}_A$ and $\mathcal{H}_B$ we obtain outcomes $a \in A$ and $b \in B$ given measurement settings $s \in S$ and $t \in T$ respectively. Furthermore, let $m^{AB}(a,s,b|t)$ denote the joint probability of obtaining outcomes $a$ and $b$ given settings $s$ and $t$ when performing measurements on systems $\mathcal{H}_A$ and $\mathcal{H}_B$.

Informally, our question is now: Given probabilities $m^{AB}(a|s,b|t)$, does there exist a shared state $\rho$ such that we can find measurements on the individual systems $\mathcal{H}_A$ and $\mathcal{H}_B$ that lead to such probabilities? Let’s first consider what polynomial equations and inequalities we need to express our problem in the above form. First of all, how can we express the fact that we want our measurement operators to act on the individual systems $\mathcal{H}_A$ and $\mathcal{H}_B$ alone? I.e., how can we ensure that the measurement operators have tensor product form? We will show in Lemma 4.1 that we
are guaranteed to observe such a tensor product form if and only if for all \( s \in S, \ a \in A, \ t \in T \) and \( b \in B \) we have \([A^a_s, B^b_t] = 0\), where we used \( A^a_s \) and \( B^b_t \) to denote the measurement operators of Alice and Bob corresponding to measurement settings \( s \) and \( t \) and outcomes \( a \) and \( b \) respectively. Hence, we need to impose the polynomial equality constraints of the form \([A^a_s, B^b_t] = 0\).

Furthermore, we want that for both systems \( A \) and \( B \), we obtain a valid measurement for each measurement setting \( s \in S \) and \( t \in T \). I.e., we impose further polynomial equality constraints for all \( s \in S \) and \( t \in T \) of the form

\[
\sum_{a \in A} A^a_s - I = 0 \quad \text{and} \quad \sum_{b \in B} B^b_t - I = 0,
\]

and finally the following polynomial inequality constraints for all \( a \in A \) and \( b \in B \)

\[
A^a_s \geq 0 \quad \text{and} \quad B^b_t \geq 0.
\]

Recall, that we may restrict ourselves to considering projective measurements. We may thus add the equality constraints

\[
(A^a_s)^2 = A^a_s \quad \text{and} \quad (B^b_t)^2 = B^b_t,
\]

which automatically imply that \( A^a_s, B^b_t \geq 0 \). For simplicity, we will later use this constraint instead of the previous one.

In this paper, we are mainly concerned with the (weighted) average of the probabilities of generating certain outcomes in a non-local game. In other words, we wanted to know if there exist operators of the above form such that

\[
\nu = \left\| \sum_{a,b,s,t} \pi(s,t) V(a,b|s,t) A^a_s B^b_t \right\|
\]

for some success probability \( \nu \). Semidefinite programming will allow us to turn the question of existence into an optimization problem.

4 Tools

For our analysis we first need to introduce two key tools. The first one allows us to deal with the fact that we want measurements to have tensor product form. Our second tool is an extension of the non-commutative Positivstellensatz of Helton and McCullough to the field of complex numbers, from which we will derive a converging hierarchy of semidefinite programs.

4.1 Tensor product structure from commutation relations

We now first show that imposing commutativity constraints does indeed give us the tensor product structure required for our analysis of non-local games. It is well-known that the following statement holds within the framework of quantum mechanics \(^2\).

\[^2\text{an algebra of type-I}\]

In Appendix \[^A\] we provide a simple version of this argument accessible from a computer science perspective, which directly applies to the task at hand.
Lemma 4.1. Let $\mathcal{H}$ be a finite-dimensional Hilbert space, and let $\{X_{s_j}^{a_j} \in \mathbb{B}(\mathcal{H}) \mid \text{for all } j \in [N] \text{ and for all } s_j \in S_j, a_j \in A_j\}$. Then the following two statements are equivalent:

1. For all $j,j' \in [N], j \neq j'$, and all $s_j \in S_j$, $s_{j'} \in S_{j'}$, $a_j \in A_j$ and $a_{j'} \in A_{j'}$ it holds that $[X_{s_j}^{a_j}, X_{s_{j'}}^{a_{j'}}] = 0$.

2. There exist Hilbert spaces $\mathcal{H}_1, \ldots, \mathcal{H}_N$ such that $\mathcal{H} = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_N$ and for all $j \in [N]$, all $s_j \in S_j$, $a_j \in A_j$ we have $X_{s_j}^{a_j} \in \mathbb{B}(\mathcal{H}_j)$.

4.2 Positivstellensatz

Our second tool, the Positivstellensatz (in combination with semidefinite programming) will allow us to find certificates for the fact a quantum moment problem is infeasible. For simplicity, we here describe the Positivstellensatz from the perspective of non-local games. An extension to the general quantum moment problem is possible and will be provided in a longer version of this paper. Our results follow almost directly from Helton and McCullough’s work and our proof closely follows that in Ref. [23]. We have chosen to provide a complete proof of the Positivstellensatz for three reasons: (i) the proof is more straightforward in our concrete setting, (ii) Helton and McCullough’s theorem is formulated for symmetric operators over the field $\mathbb{R}$, and we need to work with Hermitian operators over the field $\mathbb{C}$, and (iii) so we can highlight the nonconstructive steps in the proof. We first define:

Definition 4.2 (Convex Cone $\mathcal{C}_P$). Let $\mathcal{P}$ be a collection of Hermitian polynomials in (noncommutative) variables $\{X_{s_j}^{a_j}\}$. The convex cone $\mathcal{C}_P$ generated by $\mathcal{P}$ consists of polynomials of the form

$$q = \sum_{i=1}^{M} r_i^\dagger r_i + \sum_{i=1}^{N} \sum_{j=1}^{L} s_{ij}^\dagger p_i s_{ij},$$

where $p_i \in \mathcal{P}$, $M$, $N$ and $L$ are finite, and $r_i$, $s_{ij}$ are arbitrary polynomials.

In the following, we will call Eq. (3) a weighted sum of squares (WSOS) representation of $q$.

The purpose of the set $\mathcal{P}$ is to keep track of the constraints on the measurement operators. Note that when considering the measurement operators for non-local games, it is sufficient for us to restrict ourselves to considering (measurement) operators that are positive semidefinite. In particular, this means that all operators are Hermitian. The Positivstellensatz as such does not require us to deal only with Hermitian variables in the polynomials, but allows us to use any noncommuting matrix variables. In the following, we will always take our measurement operators to be of the form $X_s^a = (\hat{X}_s^a)^\dagger \hat{X}_s^a$. Clearly, $X_s^a$ is itself a Hermitian polynomial in the variable $\hat{X}_s^a$.

For clarity of notation, we will omit this explicit expansion in the future. Note that we will thus not impose the constraint that our operators are Hermitian, and this implicit expansion does not increase the size of our SDP.

We can write our constraints in terms of the following sets of Hermitian polynomials. In the following, we will use the short hand notation $O_{-j} := X_{s_1}^{a_1} \ldots X_{s_{j-1}}^{a_{j-1}} X_{s_{j+1}}^{a_{j+1}} \ldots X_{s_N}^{a_N}$ where we leave indices $s_j$ and $a_j$ implicit, to refer to a product of measurement operators where we exclude player $j$. First, we want measurements on different subsystems to commute. In the multi-party case, this gives us the set of polynomials

$$\mathcal{Q}_1 = \{i[X_{s_j}^{a_j}, O_{-j}] \mid \text{for all } s_j \in S_j, a_j \in A_j \text{ and all } O_{-j}\}.$$
Second, we want our operators to form valid measurements. 

$$Q_2 = \bigcup_{j,s_j} \{ I - \sum_{a_j} X_{s_j}^{a_j} \}.$$ 

Finally, by Neumark’s theorem [40], we may take our measurement operators to be projectors, this gives 

$$Q_3 = \bigcup_{j,s_j,a_j} \{ (X_{s_j}^{a_j})^2 - X_{s_j}^{a_j} \}.$$ 

It’s not hard to see that these constraints actually give us orthogonality of the projectors. For clarity, however, we may also include the following sets of polynomials 

$$Q_4 = \{ i[X_{s_j}^{a_j}, X_{s_j}^{a'_j}] \mid \text{for all } s_j \in S_j \text{ and all } a_j \neq a'_j \},$$ 

$$Q_5 = \{ X_{s_j}^{a_j} X_{s_j}^{a'_j} + X_{s_j}^{a'_j} X_{s_j}^{a_j} \mid \text{for all } s_j \in S_j \text{ and all } a_j \neq a'_j \},$$ 

which explicitly demand that projectors corresponding to the same $s_j$ are orthogonal.

Let $Q = Q_1 \cup Q_2 \cup Q_3 \cup Q_4 \cup Q_5$ and let $P = Q \cup (-Q)$. Note that all polynomials in $P$ are Hermitian. It is clear that if the measurement operator satisfy the constraints, then the term 

$$\sum_{i,j} s_{ij}^\dagger p_j s_{ij}$$ 

vanishes for arbitrary $p_j \in P$ and arbitrary polynomial $s_{ij}$. We are now ready to state the Positivstellensatz:

**Theorem 4.3** (Positivstellensatz). Let $G = G(\pi, V)$ be an $N$-prover game and let $C_P$ be the cone generated by the set $P$ defined above. Set 

$$q_\nu = \nu I - \sum_{s_1, \ldots, s_N} \pi(s_1, \ldots, s_N) \sum_{a_1, \ldots, a_N} V(a_1, \ldots, a_N | s_1, \ldots, s_N) X_{s_1}^{a_1} \ldots X_{s_N}^{a_N}. \quad (4)$$ 

If $q_\nu > 0$, then $q_\nu \in C_P$, i.e., 

$$\nu I - \sum_{s_1, \ldots, s_N} \pi(s_1, \ldots, s_N) \sum_{a_1, \ldots, a_N} V(a_1, \ldots, a_N | s_1, \ldots, s_N) X_{s_1}^{a_1} \ldots X_{s_N}^{a_N} = \sum_{i} r_i^\dagger r_i + \sum_{i,j} s_{ij}^\dagger p_i s_{ij}, \quad (5)$$ 

for some $p_i \in P$, and some polynomials $r_i, s_{ij}$.

### 5 Finding upper bounds

We now show how we can approximate the optimal field-theoretic value of a non-local game using semidefinite programming. We thereby construct a converging hierarchy of SDPs, where each level in this hierarchy gives us a better upper bound on the actual value of the game. To this end we will use the Positivstellensatz of Theorem 4.3 in combination with the beautiful approach of Parrilo [38, 39]. For simplicity, we first describe everything for the two party setting; a generalization is straightforward.
Recall from Definition 2.2 that if for some real number $\nu$ we have

$$ q_\nu = \nu I - \sum_{a,b,s,t} \pi(s,t) V(a,b|s,t) A_s^a B_t^b \geq 0, \quad (6) $$

and the operators $\{A_s^a\}$ and $\{B_t^b\}$ form a valid measurement, then $\nu \geq \omega^f(G)$ gives us an upper bound for the optimum value of the game. When trying to find the optimal value of the game, our task is thus to find the smallest $\nu$ for which $q_\nu \geq 0$ for any choice of measurement operators. Clearly, if we could express $q_\nu$ as an SOS for any choice of measurement operators $\{A_s^a\}$ and $\{B_t^b\}$ then $q_\nu \geq 0$ and we would also have $\nu \geq \omega^f(G)$. Luckily, the Positivstellensatz of Theorem 4.3 gives us almost the converse: if $q_\nu > 0$, then $q_\nu$ can be written as a weighted sum of squares (WSOS). Recall from the previous section, that the purpose of the additional term in the weighted sums of squares representation is to deal with the constraint that we would like the operators $\{A_s^a\}$ and $\{B_t^b\}$ to form a valid quantum measurement. Note that $q_\nu$ reduces to an SOS if we could express $q_\nu$ as a WSOS, i.e.,

$$ q_\nu = \nu I - \sum_{a,b,s,t} \pi(s,t) V(a,b|s,t) A_s^a B_t^b = M \sum_{i=1} r_i \dagger r_i + N \sum_{i=1} \sum_{j=1} s_{ij} \dagger p_i s_{ij}, \quad (7) $$

for some polynomials $r_i$ and $s_{ij}$ in the variables $\{A_s^a\}$ and $\{B_t^b\}$ in such a way that whenever the variables satisfy the constraints the second term in the above expansion vanishes.

It is not difficult to see that if $q_\nu > 0$, then there exists no strategy that achieves a winning probability of $\nu$ or higher. Applied to our problem, the Positivstellensatz thus tells us that if there exists no strategy that achieves winning probability $\nu$, then $q_\nu$ can be written as a weighted sum of squares. Intuitively, the WSOS representation of $q_\nu$ thus bears witness to the fact that the set of measurement operators and states giving a success probability higher than $\nu$ is empty. The advantage of this procedure is that semidefinite programming can be used to test whether polynomials (such as $q_\nu$) admit a representation as WSOS. In Section 5.2, we will look at some specific examples of this approach (see also [39, 43] for the analogous treatment for commutative variables).

When trying to find the optimal value of the game, our task is thus to find the smallest $\nu$ for which $q_\nu$ admits a WSOS representation. Hence, we want to

$$ \begin{align*}
\text{minimize} & \quad \nu \\
\text{subject to} & \quad q_\nu \in C_P.
\end{align*} $$

Recall that if $q_\nu \in C_P$, then $q_\nu$ is of the form

$$ q_\nu = \sum_{i=1}^M r_i \dagger r_i + \sum_{i=1}^N \sum_{j=1}^L s_{ij} \dagger p_i s_{ij}, \quad (8) $$

for some polynomials $r_i$ and $s_{ij}$ in the variables $\{A_s^a\}$ and $\{B_t^b\}$. A point that is worth noting now is that in the above optimization, Eq. (8) is an identity true for all $\{A_s^a\}$, $\{B_t^b\}$, rather than an equation that is only true when $\{A_s^a\}$, $\{B_t^b\}$ correspond to projective measurements. In this, the additional term is rather similar to the Lagrange multipliers in more conventional constrained optimizations.
5.1 SDP hierarchy

The main difficulty now is that we do not know how large the WSOS representation of \( q_\nu \) has to be. That is, we do not know ahead of time how large we need to choose the degree of the polynomials in the representation. The techniques discussed above are therefore not constructive and do not lead to a direct computation of \( \omega^f(G) \). However it is straightforward to find semidefinite relaxations that provide upper bounds on \( \omega^f(G) \). In this we simply apply the methods of Parrilo \[38, 39\] for the case of polynomials of commutative variables. The main requirement is to fix an integer \( n \) and look for a sum of squares decomposition for \( q_\nu \) that has a total degree of at most \( 2n \). Letting \( \nu = \omega^f(G) + \varepsilon \), this means that \( \varepsilon \) may not be made arbitrarily small but will always result in an upper bound for \( \omega^f(G) \). This upper bound can be computed as an SDP using methods analogous to \[39\]. Consider the problem given above for \( q_\nu \) as in Eq. (8). Notice that all of the constraint polynomials \( p_i \) defined in Section 4.2 have total degree less than or equal to 2 so we require that each \( r_i \) is of total degree \( n \) and each \( s_i \) is of total degree at most \( n - 1 \). The lowest level of the hierarchy has \( n = 1 \) and corresponds to applying the method of Lagrange multipliers to finding the quantum value of the game. In the following, we use the term level \( n \) to refer to a level of the hierarchy where the total degree of \( q_\nu \) is \( 2n \) when concerned with a bipartite game. For a game \( G \), denote the solution to the SDP at level \( n \) as \( \omega^{sdp}_n(G) \). It should be clear that if \( q_\nu \) has a WSOS decomposition of degree \( 2n \), it must also have a WSOS decomposition with higher degree. As such, the optimum derived from the hierarchy of SDPs must obey the following inequalities:

\[ \omega^{sdp}_1(G) \geq \omega^{sdp}_2(G) \geq \cdots \geq \omega^{sdp}_n(G). \]  

(9)

**Theorem 5.1.** The solutions to the SDP hierarchy converge to \( \omega^f(G) \), i.e., \( \lim_{n \to \infty} \omega^{sdp}_n = \omega^f(G) \).

**Proof.** That \( \omega^{sdp}_n(G) \geq \omega^f(G) \) follows from our discussion above. To prove convergence, we use the Positivstellensatz given by Theorem 4.3. Fix \( \varepsilon > 0 \) and let \( \nu = \omega^f(G) + \varepsilon \) with \( q_\nu \) defined as in Eq. (4). By Theorem 4.3, \( q_\nu \) has a representation as a WSOS,

\[ q_\nu = \sum_{i=1}^M r_i^\dagger r_i + \sum_{i=1}^N \sum_{j=1}^L s^\dagger_{ij} p_i s_{ij}, \]

Let \( 2D \) be the maximum degree of any of the polynomials \( r_i^\dagger r_i \) and \( s^\dagger_{ij} p_i s_{ij} \) that occurs in the above expression. Then, if we consider a level \( D \) SDP relaxation, we must necessarily arrive at an optimum such that \( \omega^{sdp}_D(G) \leq \omega^f(G) + \varepsilon \). Likewise, by choosing \( \varepsilon \) arbitrarily close to zero, there is a corresponding SDP with total degree \( 2n \) whose optimum \( \omega^{sdp}_n(G) \) is arbitrarily close to \( \omega^f(G) \). In particular, from Eq. (9), we can see that as \( n \to \infty \), the optimum of the SDP hierarchy must converge to \( \omega^f(G) \). \( \square \)

In Section 5.2.2 we provide a simple example of how the degree of the polynomials can be increased when going from level 1 to level 2. There are many connections of this semidefinite programming hierarchy to other methods that can be used to bound the quantum values of games. In particular, it can be shown that the dual semidefinite programs to this hierarchy are equivalent to the moment matrix methods of NPA \[36\], thus showing that the hierarchy of semidefinite programs discussed in that work converges to the entangled value of the game. Our example of the CHSH inequality below demonstrates this connection explicitly. In relation to this, it is worth noting that the duality between the two approaches (sum of squares and moment matrix) arises also in the
case of commutative variables where the moment matrix methods of Laserre [30] are dual to the semidefinite programs discussed by Parrilo [39].

5.2 Examples

5.2.1 CHSH inequality

We will now look at the simplest non-local game that is derived from the CHSH inequality [14]. In particular, we will illustrate how the tools that have we developed allow us to prove that

$$S_{\text{CHSH}} = \langle A_1 B_1 \rangle + \langle A_1 B_2 \rangle + \langle A_2 B_1 \rangle - \langle A_2 B_2 \rangle \leq 2\sqrt{2},$$

where $A_1, A_2$ and $B_1, B_2$ are observables with eigenvalues $\pm 1$ corresponding to Alice and Bob’s measurement settings respectively. First of all, note that since we are only interested in the expectation values of the form $\langle A_1 B_2 \rangle$ we may simplify our problem: instead of dealing with the probabilities of individual measurement outcomes, we are only interested in whether said expectation values can be obtained. Here, our constraints become much simpler and we only demand that $A_j^2 = I, B_j^2 = I$ and $[A_j, B_k] = 0$ for all $j, k \in \{1, 2\}$. The Bell operator for the CHSH inequality is given by [8]

$$B_{\text{CHSH}} = A_1 B_1 + A_1 B_2 + A_2 B_1 - A_2 B_2.$$ 

Hence, to find the optimum value our goal is to

$$\text{minimize } \nu \text{ subject to } q_\nu = \nu I - B_{\text{CHSH}} \in \mathcal{C}_P.$$ 

The constraint in the above optimization thereby amounts to determining whether $q_\nu$ as written above can be cast in the form of a WSOS, which reduces to an SOS for measurement operators satisfying the constraints. The numerical package SOSTOOLS [42] gives a frontend to other SDP solvers and explains how to apply these techniques in the case of commutative variables. Similar ideas can be applied here. However, for our simple example, it is not hard to see how this problem can be recast in a language that may be more familiar.

Since $B_{\text{CHSH}}$ is a noncommutative polynomial of degree 2, the lowest level relaxation consists of looking for a WSOS decomposition for $q_\nu$ that is of degree 2. To this end, we shall consider a vector of monomial of degree 1, namely, $z = (A_1, A_2, B_1, B_2)^\dagger$. Our goal is to find a $4 \times 4$ matrix $\Gamma$ such that $q_\nu = z^\dagger \Gamma z$ whenever the constraints are satisfied. I.e. we have $[A_j, B_k] = 0$ for all $j, k \in \{1, 2\}$, and polynomials

$$p_j^{(A)} := I - (A_j)^2, \quad p_j^{(B)} := I - (B_j)^2, \quad j = 1, 2,$$

and their negations vanish. Evidently, since we want $q_\nu$ to be a Hermitian polynomial, and we want our commutation constraints to hold, we may without loss of generality take $\Gamma$ to be real and symmetric. Note that this already takes care of the commutation constraints. Moreover, since all remaining constraints are quadratic, when looking for a WSOS decomposition for $q_\nu$, it suffices to consider $s_{ij}$ in Eq. [5] as multiples of $I$. Let $\gamma_{ij} = |\Gamma|_{i,j}$, then a small calculation shows that this amounts to requiring

$$\nu = \gamma_{11} + \gamma_{22} + \gamma_{33} + \gamma_{44},$$

$$0 = \gamma_{12} = \gamma_{21} = \gamma_{34} = \gamma_{43},$$

$$-1 = 2\gamma_{13} = 2\gamma_{14} = 2\gamma_{23},$$

$$1 = 2\gamma_{24},$$

(11)
so that

\[ q_\nu = \nu I - B_{\text{CHSH}} = z^\dagger \Gamma z + \sum_{j=1}^{2} \gamma_{jj} p_j(A) + \sum_{j=3}^{4} \gamma_{jj} p_j(B). \]  

(12)

Using the constraints given in Eq. (11), we see that \( \Gamma \) should be of the form

\[ \Gamma = \frac{1}{2} \begin{pmatrix} 
2\gamma_{11} & 0 & -1 & -1 \\
0 & 2\gamma_{22} & -1 & 1 \\
-1 & -1 & 2\gamma_{33} & 0 \\
-1 & 1 & 0 & 2\gamma_{44} 
\end{pmatrix}. \]  

(13)

Effectively, \( \Gamma \) is the matrix obtained by expressing \( \nu I - B_{\text{CHSH}} - \sum_{j=1}^{2} \gamma_{jj} p_j(A) - \sum_{j=3}^{4} \gamma_{jj} p_j(B) \) in the form of \( z^\dagger \Gamma z \). Now, if we can find a \( \Gamma \geq 0 \) that is of this form, then whenever the polynomials given in Eq. (10) vanish, \( q_\nu = z^\dagger \Gamma z \) is an SOS. To see this, note that in this case, we may write \( \Gamma = U^\dagger DU \), where \( U \) is unitary and \( D = \text{diag}(d_i) \) only consists of nonnegative diagonal entries. Then we can write \( q_\nu \) as \( \sum_i d_i (Uz)^\dagger_i (Uz)_i \) which is clearly an SOS. Conversely, note that if \( q_\nu \) is an SOS, we can find such a matrix \( \Gamma \). Hence, we can rephrase our optimization problem as the SDP

\[
\begin{align*}
\text{minimize} & \quad \text{Tr}(\Gamma) \\
\text{subject to} & \quad \Gamma \geq 0.
\end{align*}
\]

This is, in fact, exactly the dual of the SDP corresponding to the first level of the SDP hierarchy given by NPA \[36\], and the dual of the SDP for the special case of XOR games \[49\]. Solving this SDP, one obtains

\[ \Gamma = \frac{1}{2} \begin{pmatrix} \sqrt{2} & 0 & -1 & -1 \\
0 & \sqrt{2} & -1 & 1 \\
-1 & -1 & \sqrt{2} & 0 \\
-1 & 1 & 0 & \sqrt{2} \end{pmatrix}, \]  

(14)

which gives \( 2\sqrt{2} \) as an optimum. From here and Eq. (12), it is possible to write down a WSOS decomposition for \( \nu = 2\sqrt{2} \) as

\[ q_{2\sqrt{2}} = 2\sqrt{2} I - B_{\text{CHSH}} = \frac{1}{2\sqrt{2}} (h_1^\dagger h_1 + h_2^\dagger h_2) + \frac{1}{\sqrt{2}} \sum_{j=1}^{2} p_j(A) + \frac{1}{\sqrt{2}} \sum_{j=3}^{4} p_j(B), \]  

(15)

with \( h_1 = A_1 + A_2 - \sqrt{2} B_1 \) and \( h_2 = A_1 - A_2 - \sqrt{2} B_2 \). This immediately implies that whenever the constraints are satisfied, \( q_{2\sqrt{2}} \geq 0 \) and hence \( B_{\text{CHSH}} \leq 2\sqrt{2} I \). It is well known that for the CHSH inequality, this bound can be achieved \[11\].

### 5.2.2 The \( I_{3322} \) inequality

We now consider another example of a two-player game, where the first level of the hierarchy does not give a tight bound. The \( I_{3322} \) inequality \[16\] is a Bell inequality phrased in terms of probabilities (not expectation values) whereby Alice and Bob can each perform one of three possible two-outcome measurements. Without loss of generality, the Bell operator in this case can be written as:

\[ B_{3322} = A_1^b (B_1^b + B_2^b + B_3^b) + A_2^b (B_1^b + B_2^b - B_3^b) + A_3^b (B_1^b - B_2^b) - A_1^c - 2B_1^b - B_2^b, \]

16
where \( A^a_i \) and \( B^b_j \) \((i, j = 1, 2, 3)\) are projectors corresponding to, respectively, outcome \( a \) of Alice’s \( i \)-th measurement and outcome \( b \) of Bob’s \( j \)-th measurement for some fixed \( a \) and \( b \). To the best of our knowledge, the maximum entangled value for \( B_{3322} \), i.e., \( \omega^*(I_{3322}) \), is not known. The best known lower bound on \( \omega^*(I_{3322}) \) is 0.25 \( [10] \); some upper bounds (0.375 \( [31] \), 0.3660 \( [1] \)) are also known in the literature. Here, we will make use of the tools that we have developed to obtain a hierarchy of upper bounds on this maximum. In analogous with the CHSH scenario, this corresponds to solving the following SDP for some fixed degree of \( q_\nu \):

\[
\begin{align*}
\text{minimize} & \quad \nu, \\
\text{subject to} & \quad q_\nu = \nu \mathbb{I} - B_{3322} \in C_\mathbb{P}.
\end{align*}
\]

(16)

In particular, since \( B_{3322} \) is a noncommutative polynomial of degree 2, the lowest level SDP relaxation would correspond to choosing a vector of monomials with degree at most one, i.e.,

\[
z^\dagger = (\mathbb{I}, A^a_1, A^a_2, A^a_3, B^b_1, B^b_2, B^b_3).
\]

(17)

We can now proceed analogously to the CHSH case, where we will look for a particular matrix \( \Gamma \) restricted by our constraints, namely, \((A^a_j)^2 = A^a_j\) and \((B^b_j)^2 = B^b_j\) for all \( j \in \{1, 2, 3\} \), where again for the purpose of implementation, we will implicitly enforce the commutativity conditions \([A_i, B_j] = 0\) for all \( i, j \in \{1, 2, 3\} \). Solving the corresponding SDP (Appendix \( [D.1] \)), one obtains \( \omega_1^{\mathrm{sdp}}(I_{3322}) = 3/8 \), and the matrix

\[
\Gamma = \frac{1}{2} \begin{pmatrix}
\frac{3}{4} & 0 & -1 & \frac{1}{2} & 1 & 0 & -\frac{1}{2} \\
0 & 2 & 0 & 0 & -1 & -1 & -1 \\
-1 & 0 & 2 & 0 & -1 & -1 & 1 \\
-\frac{1}{2} & 0 & 0 & 1 & -1 & 1 & 0 \\
1 & -1 & -1 & -1 & 2 & 0 & 0 \\
0 & -1 & -1 & 1 & 0 & 2 & 0 \\
-\frac{1}{2} & -1 & 1 & 0 & 0 & 0 & 1
\end{pmatrix},
\]

which provides a WSOS decomposition for \( \nu = 3/8 \), i.e.,

\[
q_{3/8} = \frac{3}{8} \mathbb{I} - B_{3322} = z^\dagger \Gamma z + \sum_i s_i^\dagger p_i s_i,
\]

(18)

where

\[
p_i = \begin{cases}
A^a_i - (A^a_i)^2 & : i = 1, 2, 3, \\
B^b_{i-3} - (B^b_{i-3})^2 & : i = 4, 5, 6,
\end{cases}
\quad s_i = \begin{cases}
1 & : i = 1, 2, 4, 5, \\
\frac{1}{\sqrt{2}} & : i = 3, 6.
\end{cases}
\]

(19)

Given that \( \omega_1^{\mathrm{sdp}}(I_{3322}) \) is far from the best known lower bound on \( \omega^*(I_{3322}) \), it seems natural to also look at higher level relaxations for \( I_{3322} \). For the next level, we will look for \( q_\nu \) that is of degree at most 4. Note that we have many options to extend the hierarchy. The easiest way to proceed is to extend the vector \( z \) by some monomials of degree two in the measurement operators. For this we do not even have to consider using all possible degree 2 monomials, but could consider only a subset of them such as that given by the following vector

\[
z^\dagger = (\mathbb{I}, A^a_1, A^a_2, A^a_3, B^b_1, B^b_2, B^b_3, A^a_1 B^b_1, A^a_2 B^b_2, A^a_3 B^b_3, A^a_1 B^b_1, A^a_2 B^b_2, A^a_3 B^b_3, A^a_1 B^b_1, A^a_2 B^b_2, A^a_3 B^b_3).
\]

(20)
In particular, solving the corresponding SDP (Appendix [D.2]) with \( z \) given by Eq. (20) gives an optimum that is approximately 0.251 470 90 which is significantly less than \( 3/8 = 0.375 \). Clearly, we could increase the size of \( z \) further by including all relevant monomials of degree 2 or less.

\[
z^\dagger = (\mathbb{I}, A_1^a, A_2^a, \ldots, B_1^b, B_2^b, A_1^a A_2^a, A_1^a A_3^a, \ldots, A_3^a A_2^a, B_1^b B_2^b, B_1^b B_3^b, \ldots, B_2^b B_3^b, A_1^b B_1^b, A_1^b B_2^b, A_1^b B_3^b, \ldots, A_3^b B_3^b).
\]

Proceeding as before, we end up with the optimum of the second order relaxation \( \omega_2^{\text{sdp}}(I_{3322}) \approx 0.250\ 939\ 72 \). In the next level, we would then include all monomials of degree 3 and less, and this gives \( \omega_3^{\text{sdp}}(I_{3322}) \approx 0.250\ 875\ 56 \).

5.2.3 Yao’s inequality

Finally, we examine a well-known tripartite Bell inequality [50] among three provers: Alice, Bob and Charlie. Each prover performs three possible measurements, each of which has two possible outcomes. Similarly to the CHSH inequality above, we may thus express each measurement as an observable with eigenvalues \( \pm 1 \). For simplicity, let \( A_1, A_2, A_3, B_1, B_2, B_3 \) and \( C_1, C_2, C_3 \) correspond to the observables of Alice, Bob and Charlie respectively. Yao’s inequality states that for any shared state \( \rho \) we have

\[
\mathcal{S}_{\text{Yao}} = \langle A_1 B_2 C_3 \rangle + \langle A_2 B_3 C_1 \rangle + \langle A_3 B_1 C_2 \rangle - \langle A_1 B_3 C_2 \rangle - \langle A_2 B_1 C_3 \rangle - \langle A_3 B_2 C_1 \rangle \leq 3\sqrt{3}.
\]  

(21)

We now provide a very simple proof of this inequality based on our framework. First of all, note that since we are only interested in the expectation values of the form \( \langle A_1 B_2 C_3 \rangle \) we may again restrict ourselves to dealing only with expectation values in analogy with the CHSH example presented above. Our constraints are also analogous to the CHSH case. Among them, we have the following constraint polynomials

\[
p_j^{(A)} := \mathbb{I} - (A_j)^2, \quad p_j^{(B)} := \mathbb{I} - (B_j)^2, \quad p_j^{(C)} := \mathbb{I} - (C_j)^2,
\]

for \( j = 1, 2, 3 \). Next, note that the Bell operator for Yao’s inequality can be written as [c.f. Eq. (21)]

\[
\mathcal{B}_{\text{Yao}} = A_1 B_2 C_3 + A_2 B_3 C_1 + A_3 B_1 C_2 - A_1 B_3 C_2 - A_2 B_1 C_3 - A_3 B_2 C_1,
\]

(23)

which is a noncommutative polynomial of degree 3.

For our task at hand, we will consider the following SDP relaxation

\[
\text{minimize} \quad \nu,
\]

subject to \( q_\nu = \nu \mathbb{I} - \mathcal{B}_{\text{Yao}} \in C_\mathcal{P} \),

with \( q_\nu \) being a polynomial of degree at most 6. As usual, we will implicitly enforce the commutativity constraints, i.e., \( [A_i, B_j] = 0, [A_i, C_k] = 0 \), and \( [B_j, C_k] = 0 \) for all \( i, j, k \in \{1, 2, 3\} \). With this assumption, it turns out that it suffices to consider the following 25-element vector

\[
z = \left( \begin{array}{c}
\mathbb{I} \\
A_1 B_2 C_3 \\
A_2 B_3 C_1 \\
A_3 B_1 C_2 \\
A_1 B_3 C_2 \\
A_2 B_1 C_3 \\
A_3 B_2 C_1 \\
A_1 B_2 C_1 \\
A_1 B_3 C_1 \\
A_2 B_3 C_1 \\
A_3 B_1 C_1 \\
A_1 B_2 C_2 \\
A_1 B_3 C_2 \\
A_2 B_3 C_2 \\
A_3 B_1 C_2 \\
A_1 B_2 C_3 \\
A_1 B_3 C_3 \\
A_2 B_3 C_3 \\
A_3 B_1 C_3 \\
A_2 B_1 C_3 \\
A_3 B_2 C_3 \\
A_3 B_2 C_1 \\
A_3 B_3 C_1 \\
A_2 B_3 C_2 \\
A_3 B_3 C_2 \\
A_3 B_3 C_1
\end{array} \right) \oplus \left( \begin{array}{c}
A_1 B_1 C_2 \\
A_1 B_2 C_1 \\
A_1 B_3 C_1 \\
A_2 B_2 C_1 \\
A_2 B_3 C_1 \\
A_3 B_2 C_1 \\
A_2 B_1 C_2 \\
A_2 B_3 C_2 \\
A_3 B_1 C_2 \\
A_3 B_2 C_2 \\
A_3 B_3 C_2 \\
A_2 B_1 C_3 \\
A_2 B_2 C_3 \\
A_2 B_3 C_3 \\
A_3 B_1 C_3 \\
A_3 B_2 C_3 \\
A_3 B_3 C_3 \\
A_2 B_1 C_2 \\
A_2 B_2 C_2 \\
A_2 B_3 C_2 \\
A_3 B_1 C_2 \\
A_3 B_2 C_2 \\
A_3 B_3 C_2 \\
A_2 B_1 C_3 \\
A_2 B_2 C_3 \\
A_2 B_3 C_3 \\
A_3 B_1 C_3 \\
A_3 B_2 C_3 \\
A_3 B_3 C_3
\end{array} \right) \oplus \left( \begin{array}{c}
A_2 B_2 C_3 \\
A_2 B_3 C_2 \\
A_3 B_2 C_2 \\
A_3 B_3 C_2 \\
A_3 B_2 C_3 \\
A_3 B_3 C_3
\end{array} \right).
\]  

(24)
In this case, since the constraint polynomials given in Eq. (22) are quadratic, when looking for a WSOS decomposition for \( q_{ij} \), we will need to consider \( s_{ij} \) in Eq. (8) as an arbitrary polynomial of \( A_i, B_j \) and \( C_k \) with degree at most 2. Proceeding in a way analogous to the 2nd level relaxation for \( I_{3322} \) inequality, one obtains the \( 25 \times 25 \) positive semidefinite matrix \( \Gamma = \Gamma_{7 \times 7} \bigoplus_{i=1}^{6} \Gamma_{3 \times 3} \), where

\[
\Gamma_{7 \times 7} := \frac{1}{2} \begin{pmatrix}
3\sqrt{3} & -1 & -1 & -1 & 1 & 1 & 1 \\
-1 & \frac{1}{\sqrt{3}} & 0 & 0 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
-1 & 0 & \frac{1}{\sqrt{3}} & 0 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
-1 & 0 & 0 & \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
1 & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} & 0 \\
1 & -\frac{3}{\sqrt{3}} & -\frac{3}{\sqrt{3}} & -\frac{3}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{3}} \\
1 & -\frac{3}{\sqrt{3}} & -\frac{3}{\sqrt{3}} & -\frac{3}{\sqrt{3}} & 0 & 0 & \frac{1}{\sqrt{3}} \\
\end{pmatrix}, \quad \Gamma_{3 \times 3} := \frac{1}{12\sqrt{3}} \begin{pmatrix}
1 & 1 & 1 \\
1 & 1 & 1 \\
1 & 1 & 1 \\
\end{pmatrix}.
\]

(25)

From some simple calculations, it then follows that whenever the constraints \( A_i^2 = B_j^2 = C_k^2 = 1 \) are satisfied, we have

\[
3\sqrt{3} I - B_{\text{Yao}} = z^\dagger \Gamma z = \frac{1}{6\sqrt{3}} \left( h_0^\dagger h_0 + \sum_{j=1}^{2} h_{+,j}^\dagger h_{+,j} + \sum_{j=1}^{2} h_{-,j}^\dagger h_{-,j} + \frac{1}{2} \sum_{j,k=1,2,3} h_{j,k}^\dagger h_{j,k} \right),
\]

(26)

where

\[
\begin{align*}
h_0 &= 3\sqrt{3} I - B_{\text{Yao}}, \\
h_{+,j} &= A_1 B_2 C_3 + e^{i(2\pi j/3)} A_2 B_3 C_1 + e^{i(4\pi j/3)} A_3 B_1 C_2, \\
h_{-,j} &= A_1 B_3 C_2 + e^{i(2\pi j/3)} A_2 B_1 C_3 + e^{i(4\pi j/3)} A_3 B_2 C_1, \\
h_{j,k} &= A_j B_j C_k + A_j B_k C_j + A_k B_j C_j.
\end{align*}
\]

This makes it explicit that whenever the constraints are satisfied, \( 3\sqrt{3} I - B_{3322} \geq 0 \) and therefore \( S_{3322} \leq 3\sqrt{3} \). As a last remark, we note that the constraint term \( \sum_{i,j} s_{ij} p_i s_{ij} \) could have been included explicitly in the WSOS decomposition for \( q_{3\sqrt{3}} = 3\sqrt{3} I - B_{\text{Yao}} \) and we refer the reader to Appendix \( D.3 \) for details.

6 Acknowledgements

We thank Stefano Pironio and Tsuyoshi Ito for interesting discussions and for sharing drafts of their papers \[34, 24\] with us. SW is supported by the National Science Foundation under contract number PHY-0456720.

References

[1] D. Avis, H. Imai, and T. Ito. On the relationship between convex bodies related to correlation experiments with dichotomic observables. *Journal of Physics A-Mathematical and General*, 39(36):11283–11299, 2006.
L. Babai. Trading group theory for randomness. In Proceedings of 17th ACM STOC, pages 421–429, 1985.

L. Babai, L. Fortnow, and C. Lund. Non-deterministic exponential time has two-prover interactive protocols. Computational Complexity, 1(1):3–40, 1991.

J. S. Bell. On the Einstein-Podolsky-Rosen paradox. Physics, 1:195–200, 1964.

M. Ben-Or, S. Goldwasser, J. Kilian, and A. Wigderson. Multi prover interactive proofs: How to remove intractability. In Proceedings of 20th ACM STOC, pages 113–131, 1988.

Stephen Boyd and Lieven Vandenberghe. Convex Optimization. Cambridge University Press, Cambridge, 2004. Available online at [http://www.stanford.edu/~boyd/cvxbook/](http://www.stanford.edu/~boyd/cvxbook/).

O. Bratteli and D. Robinson. Operator Algebras and Quantum Statistical Mechanics I. Springer, 2002.

S. L. Braunstein, A. Mann, and M. Revzen. Maximal violation of Bell inequalities for mixed states. Physical Review Letters, 68(22):3259–3261, 1992.

H. Buhrman and S. Massar. Causality and Cirel’son bounds. Physical Review A, 72:052103, 2005.

J. Cai, A. Condon, and R. Lipton. On bounded round multi-prover interactive proof systems. In Proceedings of the Fifth Annual Conference on Structure in Complexity Theory, pages 45–54, 1990.

B. Tsirelson (Cirel’son). Quantum generalizations of Bell’s inequality. Letters in Mathematical Physics, 4:93–100, 1980.

B. Tsirelson (Cirel’son). Quantum analogues of Bell inequalities: The case of two spatially separated domains. Journal of Soviet Mathematics, 36:557–570, 1987.

B. Tsirelson (Cirel’son). Some results and problems on quantum Bell-type inequalities. Hadronic Journal Supplement, 8(4):329–345, 1993.

J. Clauser, M. Horne, A. Shimony, and R. Holt. Proposed experiment to test local hidden-variable theories. Physical Review Letters, 23:880–884, 1969.

R. Cleve, P. Høyer, B. Toner, and J. Watrous. Consequences and limits of nonlocal strategies. In Proceedings of 19th IEEE Conference on Computational Complexity, pages 236–249, 2004. quant-ph/0404076.

D. Collins and N. Gisin. A relevant two qubit Bell inequality inequivalent to the CHSH inequality. Journal of Physics A:Mathematical and General, 37(5):1775–1787, 2004.

U. Feige. On the success probability of two provers in one-round proof systems. In Proceedings of the Sixth Annual Conference on Structure in Complexity Theory, pages 116–123, 1991.

U. Feige and L. Lovász. Two-prover one-round proof systems: their power and their problems. In Proceedings of 24th ACM STOC, pages 733–744, 1992.
[19] Roy J. Glauber. The quantum theory of optical coherence. *Phys. Rev. A*, 130(6):2529–2539, 1963.

[20] S. Goldwasser, S. Micali, and C. Rackoff. The knowledge complexity of interactive proof systems. *SIAM Journal on Computing*, 1(18):186–208, 1989.

[21] Rudolf Haag. *Local Quantum Physics: Fields, Particles, Algebras*. Springer, Berlin, 2nd edition, 1996.

[22] Johan H˚astad. Some optimal inapproximability results. *J. ACM*, 48(4):798–859, 2001.

[23] J. William Helton and Scott A. McCullough. A positivstellensatz for non-commutative polynomials. *Trans. Amer. Math. Soc.*, 356(9):3721–3737, 2004.

[24] Tsuyoshi Ito, Hirotada Kobayashi, and Keiji Matsumoto. Quantum multi-prover interactive proofs and decidability. In preparation.

[25] J. Kempe, H. Kobayashi, K. Matsumoto, B. Toner, and T. Vidick. On the power of entangled provers: immunizing games against entanglement. [arXiv:0704.2903](http://arxiv.org/abs/0704.2903), 2007.

[26] J. Kempe, O. Regev, and B. Toner. The unique games conjecture with entangled provers is false. [arXiv:0710.0655](http://arxiv.org/abs/0710.0655).

[27] A. Kitaev and J. Watrous. Parallelization, amplification, and exponential time simulation of quantum interactive proof systems. In *Proceedings of 32nd ACM STOC*, pages 608–617, 2000.

[28] A. Klyachko. Quantum marginal problem and n-representability. *Journal of Physics: Conference Series*, 36(1):71, 2006.

[29] D. Lapidot and A. Shamir. Fully parallelized multi prover protocols for NEXP-time. In *Proceedings of 32nd FOCS*, pages 13–18, 1991.

[30] J. B. Lasserre. Global optimization with polynomials and the problem of moments. *Siam Journal of Optimization*, 11(3):796–817, 2001.

[31] Y.-C. Liang and A. C. Doherty. Bounds on quantum correlations in Bell-inequality experiments. *Physical Review A*, 75(4):042103, April 2007.

[32] Y.-K. Liu, M. Christandl, and F. Verstraete. N-representability is QMA-complete. *Physical Review Letters*, 98:110503, 2007.

[33] L. Masanes. Extremal quantum correlations for N parties with two dichotomic observables per site. [quant-ph/0512100](http://arxiv.org/abs/quant-ph/0512100), 2005.

[34] Miguel Navascués, Stefano Pironio, and Antonio Acín. A convergent hierarchy of semidefinite programs characterizing the set of quantum correlations. [arXiv:0803.4290](http://arxiv.org/abs/0803.4290)

[35] Miguel Navascués, Stefano Pironio, and Antonio Acín. Convergent relaxations for polynomial optimization with non-commutative variables. In preparation.

[36] Miguel Navascués, Stefano Pironio, and Antonio Acín. Bounding the set of quantum correlations. *Phys. Rev. Lett.*, 98(1):010401, 2007.
A Tool 1: Tensor product structure from commutation relations

We now provide a simple proof of Lemma A.1 from a computer science perspective that is suitable to the task at hand. For simplicity, we address the case of two-prover systems in detail, and merely sketch the extension to the multiple provers at the end. For ease of reference, we shall now reproduce the Lemma for the two-prover setting:

**Lemma A.1.** Let $\mathcal{H}$ be a finite-dimensional Hilbert space, and let $\{A_s^a \in \mathbb{B}(\mathcal{H}) \mid s \in S\}$ and $\{B_t^b \in \mathbb{B}(\mathcal{H}) \mid s \in T\}$. Then the following two statements are equivalent:

1. For all $s \in S$, $t \in T$, $a \in A$ and $b \in B$ it holds that $[A_s^a, B_t^b] = 0$. 

2. There exist Hilbert spaces $\mathcal{H}_A, \mathcal{H}_B$ such that $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and for all $s \in S$, $a \in A$ we have $A_s^a \in \mathbb{B}(\mathcal{H}_A)$ and for all $t \in T$, $b \in B$ we have $B_t^b \in \mathbb{B}(\mathcal{H}_B)$.

For our argument we will not consider individual operators, but instead look at the $C^*$-algebra of operators which is well understood in finite dimensions \([4, 6, 7]\). The $C^*$-algebra of operators $\mathcal{A} = \{A_1, \ldots, A_n\}$ consists of all complex polynomials in such operators and their conjugate transpose: if $A$ is an element of the algebra, then so is $A^\dagger$. For example, the set of all bounded operators $\mathbb{B}(\mathcal{H})$ on a Hilbert space $\mathcal{H}$ is a $C^*$-algebra. For convenience, we will also write $\mathcal{A} = \langle \mathcal{A} \rangle$ for such an algebra $\mathcal{A}$ generated by operators from the set $\mathcal{A}$. We will need the following notions: The center $\mathcal{Z}$ of an algebra $\mathcal{A}$ is the set of all elements in $\mathcal{A}$ that commute with all elements of $\mathcal{A}$, i.e., $\mathcal{Z} = \{ Z | Z \in \mathcal{A}, \forall A \in \mathcal{A} : [Z, A] = 0 \}$. If $\mathcal{A} \subseteq \mathbb{B}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$, then the commutant of $\mathcal{A}$ in $\mathbb{B}(\mathcal{H})$ is given by $\text{Comm}(\mathcal{A}) = \{ X | X \in \mathbb{B}(\mathcal{H}), \forall A \in \mathcal{A} : [X, A] = 0 \}$. Furthermore, an algebra $\mathcal{A}$ is called simple, if its only ideals\(^3\) are $\{0\}$ and $\mathcal{A}$ itself. It is easy to see that if $\mathcal{A}$ only has a trivial center, i.e., $\mathcal{Z} = \{ c1 | c \in \mathbb{C} \}$, then $\mathcal{A}$ is simple \([16]\). Finally, $\mathcal{A}$ is called semisimple if it can be decomposed into a direct sum of simple algebras.

### A.1 Optimizing non-local games

Before we show how to prove Lemma \(4.1\) we first demonstrate that when considering non-local games we can greatly simplify our problem and restrict ourselves to $C^*$-algebras that are simple. It is well known that we can decompose any finite dimensional algebra into the sum of simple algebras.

**Lemma A.2 \([16]\).** Let $\mathcal{A}$ be a finite-dimensional $C^*$-algebra. Then there exists a decomposition $\mathcal{A} = \bigoplus_j \mathcal{A}_j$, such that $\mathcal{A}_j$ is simple.

We furthermore note that for any simple algebra, the following holds:

**Lemma A.3 \([16]\).** Let $\mathcal{H}$ be a Hilbert space, and let $\mathcal{A} \subseteq \mathbb{B}(\mathcal{H})$ be simple, then there exists a bipartite partitioning of the Hilbert space $\mathcal{H}$ such that $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ and $\mathcal{A} \cong \mathbb{B}(\mathcal{H}_1) \otimes \mathbb{I}_2$.

We now show that without loss of generality, we may assume that the algebras generated by Alice and Bob’s measurement operators are in fact simple.

**Lemma A.4.** Let $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ and let $\mathcal{A} = \{ A_s^a \in \mathbb{B}(\mathcal{H}_A) \}$ and $\mathcal{B} = \{ B_t^b \in \mathbb{B}(\mathcal{H}_B) \}$ be the set of Alice and Bob’s measurement operators respectively. Let $\rho \in \mathbb{B}(\mathcal{H})$ be the state shared by Alice and Bob. Suppose that for such operators we have

$$q = \sum_{s \in S, t \in T} \pi(s, t) \sum_{a \in A, b \in B} V(a, b | s, t) \text{Tr} \left( (A_s^a \otimes B_t^b) \rho \right).$$

Then there exist measurement operators $\hat{\mathcal{A}} = \{ \hat{A}_s^a \}$ and $\hat{\mathcal{B}} = \{ \hat{B}_t^b \}$ and a state $\hat{\rho}$ such

$$q \leq \sum_{s \in S, t \in T} \pi(s, t) \sum_{a \in A, b \in B} V(a, b | s, t) \text{Tr} \left( (\hat{A}_s^a \otimes \hat{B}_t^b) \hat{\rho} \right).$$

and the $C^*$-algebra generated by $\hat{\mathcal{A}}$ and $\hat{\mathcal{B}}$ is simple.

---

\(^3\)An ideal $\mathcal{I}$ of $\mathcal{A}$ is a subalgebra $\mathcal{I} \subseteq \mathcal{A}$ such that for all $I \in \mathcal{I}$ and $A \in \mathcal{A}$, we have $IA \in \mathcal{I}$ and $AI \in \mathcal{I}$. 

---

23
Proof. Let $\mathcal{A} = \langle A \rangle$ and $\mathcal{B} = \langle B \rangle$. If $\mathcal{A}$ and $\mathcal{B}$ are simple, we are done. If not, we know from Lemma A.2 and Lemma A.3 that there exists a decomposition $\mathcal{H}_A \otimes \mathcal{H}_B = \bigoplus_{jk} \mathcal{H}^j_A \otimes \mathcal{H}^k_B$. Consider $\text{Tr}((M_A \otimes M_B)\rho)$, where $M_A \otimes M_B \in \mathcal{A} \otimes \mathcal{B}$. It follows from the above that $M_A \otimes M_B = \bigoplus_{jk} (\Pi^j_A \otimes \Pi^k_B) M_A \otimes M_B (\Pi^j_A \otimes \Pi^k_B)$, where $\Pi^j_A$ and $\Pi^k_B$ are projectors onto $\mathcal{H}^j_A$ and $\mathcal{H}^k_B$ respectively. Let $\hat{\rho} = \bigoplus_{jk} (\Pi^j_A \otimes \Pi^k_B) \rho (\Pi^j_A \otimes \Pi^k_B)$. Clearly,

$$\text{Tr}((M_A \otimes M_B)\hat{\rho}) = \text{Tr} \left( \bigoplus_{jk} (\Pi^j_A \otimes \Pi^k_B) M_A \otimes M_B (\Pi^j_A \otimes \Pi^k_B) \rho \right) = \text{Tr}((M_A \otimes M_B)\rho).$$

The statement now follows immediately by convexity: Alice and Bob can now measure $\rho \{ \Pi^j_A \otimes \Pi^k_B \}$ and recording the classical outcomes $j, k$. The new measurements will then be $\hat{A}_{a,j}^i = \Pi^j_A A^i_a \Pi^j_A$ and $\hat{B}_{b,k}^t = \Pi^k_B B^t_b \Pi^k_B$ on state $\hat{\rho}_{jk} = (\Pi^j_A \otimes \Pi^k_B) \rho (\Pi^j_A \otimes \Pi^k_B) / \text{Tr}((\Pi^j_A \otimes \Pi^k_B)\rho)$. By construction, $\mathcal{A}_{\hat{j}} = \{ \hat{A}_{a,j}^i \}$ and $\mathcal{B}_{\hat{k}} = \{ \hat{B}_{b,k}^t \}$ are simple.

Let $q_{jk}$ denote the probability that we obtain outcomes $j, k$, and let

$$r_{jk} = \sum_{s,t} \pi(s,t) \sum_{a,b} V(a,b|s,t) \text{Tr}(\hat{A}_{a,j}^i \hat{B}_{b,k}^t \hat{\rho}_{jk}).$$

Then $q = \sum_{jk} q_{jk} r_{jk} \leq \max_{jk} r_{jk}$. Let $u, v$ be such that $r_{u,v} = \max_{jk} r_{jk}$. Hence, we can skip the initial measurement and instead use measurements $\hat{A}_{a,j}^i = \hat{A}_{a,j}^i$, $\hat{B}_{b,k}^t = \hat{B}_{b,k}^t$ and state $\hat{\rho} = \hat{\rho}_{u,v}$. \hfill \Box

This easy argument also immediately tells us that when $\mathcal{A}$ and $\mathcal{B}$ are abelian, we can find a classical strategy that achieves $q$: Just perform the measurement as above. If $\mathcal{A}$ and $\mathcal{B}$ are abelian, the remaining state will be one-dimensional and hence classical.

A.2 Tensor product structure

We are now ready to prove Lemma A.4. First, we examine the case where we are given a simple algebra $\mathcal{A} \in \mathbb{B}(\mathcal{H})$, for some Hilbert space $\mathcal{H}$. We will need the following version of Schur’s lemma.

Lemma A.5. Let $Z$ be the center of $\mathbb{B}(\mathcal{H})$. Then $Z = \{ c \mathbb{1} | c \in \mathbb{C} \}$.

Proof. Let $C \in Z$ and let $d = \text{dim}(\mathcal{H})$. Let $\mathcal{E} = \{ E_{ij} | i, j \in [d] \}$ be a basis for $\mathbb{B}(\mathcal{H})$, where $E_{ij} := |i\rangle \langle j|$ is the matrix of all 0’s and a 1 at position $(i, j)$. Since $C \in Z$ and $E_{ij} \in \mathbb{B}(\mathcal{H})$ we have for all $i \in [d]$

$$CE_{ii} = E_{ii}C.$$

Note that $CE_{ij}$ (or $E_{ij}C$) is the matrix of all 0’s but the $i$th column (or row) is determined by the elements of $C$. Hence all off diagonal elements of $C$ must be 0. Now consider

$$C(E_{ij} + E_{ji}) = (E_{ij} + E_{ji})C.$$

Note that $C(E_{ij} + E_{ji})$ (or $(E_{ij} + E_{ji})C$) is the matrix in which the $i$th and $j$th columns (rows) of $C$ have been swapped and the remaining elements are 0. Hence all diagonal elements of $C$ must be equal. Thus there exists some $c \in \mathbb{C}$ such that $C = c \mathbb{1}$. \hfill \Box

Using this Lemma, we can now show that
Lemma A.6. Let $C \in \mathbb{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ be such that for all $B \in \mathbb{B}(\mathcal{H}_B)$ we have

$$[C, (\mathbb{I}_A \otimes B)] = 0$$

Then there exists an $A \in \mathbb{B}(\mathcal{H}_A)$ such that $C = A \otimes \mathbb{I}_B$.

Proof. Let $d_A = \dim(\mathcal{H}_A)$ and $d_B = \dim(\mathcal{H}_B)$. Note that we can write any $C \in \mathbb{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$ as

$$C = \begin{pmatrix}
C_{11} & \cdots & C_{1d_A} \\
\vdots & \ddots & \vdots \\
C_{d_A1} & \cdots & C_{d_Ad_A}
\end{pmatrix},$$

for $d_B \times d_B$ matrices $C_{ij}$. We have $C(\mathbb{I}_A \otimes B) = (\mathbb{I}_A \otimes B)C$ if and only if for all $i, j \in [d_A]$ $C_{ij}B = BC_{ij}$, i.e., $[C_{ij}, B] = 0$. Since this must hold for all $B \in \mathbb{B}(\mathcal{H}_B)$, we have by Lemma A.5 that there exists some $a_{ij} \in C$ such that $C_{ij} = a_{ij}\mathbb{I}_B$. Hence $C = A \otimes \mathbb{I}_B$ with $A = [a_{ij}]$. \qed

For the case that the algebra generated by Alice and Bob’s measurement operators is simple, Lemma 4.1 now follows immediately:

Proof of Lemma 4.1 if $A$ is simple. Let $A = \langle \{A^a\} \rangle \subseteq \mathbb{B}(\mathcal{H})$ be the algebra generated by Alice’s measurement operators. If $A$ is simple, it follows from Lemma A.3 that $A \cong \mathbb{B}(\mathcal{H}_A) \otimes \mathbb{I}_B$ for $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. It then follows from Lemma A.6 that for all $t \in T$ and $b \in B$ we must have $B^t_b \in \mathbb{B}(\mathcal{H}_B)$. Thus, we obtain a tensor product structure! Recall that Lemma A.4 states that for our application this is all we need.

In general, what happens if $A$ is not simple? Whereas our argument shows that there always exist measurement operations such that $A$ is simple, the solution found via optimization may not have this property. We now sketch the argument in the case where the $A$ is semisimple, which by Lemma A.2 we may always assume in the finite-dimensional case. Fortunately, we can still assume that our commutation relations leave us with a bipartite structure. We can essentially infer this from von Neumann’s famous Double Commutant Theorem [46, 7], partially stated here.

Theorem A.7. Let $A$ be a finite-dimensional $C^*$-algebra. Then there exists $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ such that

$$A \cong \bigoplus_j \mathbb{B}(\mathcal{H}_A^j) \otimes \mathbb{I}_B^j$$

and

$$\text{Comm}(A) \cong \bigoplus_j \mathbb{I}_A^j \otimes \mathbb{B}(\mathcal{H}_B^j).$$

(27)

Proof. (Sketch) We already know from Lemma A.2 that $A$ can be decomposed into a sum of simple algebras. Clearly, the RHS of Eq. (27) is an element of $\text{Comm}(A)$. To see that the LHS is contained in the RHS, consider the projection $\Pi_A^j$ onto $\mathcal{H}_A^j$. Note that $\Pi_A^j \in A$, and thus for any $X \in \text{Comm}(A)$ we have $[X, \Pi_A^j] = 0$. Hence, we can write $X = \sum_j (\Pi_A^j \otimes \mathbb{I}_B)X(\Pi_A^j \otimes \mathbb{I}_B)$, and thus we can restrict ourselves to considering each factor individually. The result then follows immediately from Lemma A.6. \qed
If we have more than two provers, the argument is essentially analogous, and we merely sketch it in the relevant case when the algebra generated by the prover’s measurements is simple, since Lemma A.4 directly extends to more than two provers as well. Suppose we have N provers \( P_1, \ldots, P_N \) and let \( \mathcal{H} \) denote their joint Hilbert space. Let \( \mathcal{A} \) be the algebra generated by all measurement operators of provers \( P_1, \ldots, P_{N-1} \) respectively. Then it follows from Lemma A.6 and Lemma A.3 that there exists a bipartite partitioning of \( \mathcal{H} \) such that \( \mathcal{H} = \mathcal{H}_1, \ldots, \mathcal{H}_N, \) and for all measurement operators \( M \) of prover \( P_N \) we have that \( M \in \mathcal{B}(\mathcal{H}_N). \) By applying Lemma A.6 recursively we obtain that there exists a way to partition the Hilbert space into subsystems \( \mathcal{H}_j = \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_N \) such that the measurement operators of prover \( P_j \) act on \( \mathcal{H}_j \) alone.

In quantum mechanics, we will always obtain such a tensor product structure from commutation relations, even if the Hilbert space is infinite-dimensional. Here, we start out with a type-I algebra, the corresponding Hilbert space and operators can then be obtained by the famous Gelfand-Naimark-Segal (GNS) construction [46], an approach which is rather beautiful in its abstraction. In quantum statistical mechanics and quantum field theory, we will also encounter factors of type-II and type-III. As it turns out, the above argument does not generally hold in this case, however, there are a number of conditions that can lead to a similar structure. Sadly, we cannot consider this case here and merely refer to the survey article by Summers [45].

**B Tool 2: Positivstellensatz**

Here, we will provide the details for the proof of Theorem 4.3. For ease of reference, we first reproduce the theorem as follows:

**Theorem B.1.** Let \( G = G(\pi, V) \) be an N-prover game and let \( \mathcal{C}_P \) be the cone generated by the set \( \mathcal{P} \) defined in Section 4.2. Set

\[
q_\nu = \nu \mathbb{I} - \sum_{s_1, \ldots, s_N} \pi(s_1, \ldots, s_N) \sum_{a_1, \ldots, a_N} V(a_1, \ldots, a_N | s_1, \ldots, s_N) X_{s_1}^{a_1} \ldots X_{s_N}^{a_N}.
\]

If \( q_\nu > 0 \), then \( q_\nu \in \mathcal{C}_P \), i.e.,

\[
\nu \mathbb{I} - \sum_{s_1, \ldots, s_N} \pi(s_1, \ldots, s_N) \sum_{a_1, \ldots, a_N} V(a_1, \ldots, a_N | s_1, \ldots, s_N) X_{s_1}^{a_1} \ldots X_{s_N}^{a_N} = \sum_i r_i^\dagger r_i + \sum_{i,j} s_{ij}^\dagger s_{ij},
\]

for some \( r_i \in \mathcal{P} \), and some polynomials \( r_i, s_{ij} \).

We now prove the contrapositive statement of Theorem B.1. In particular, we show that if \( q_\nu \) has no representation as a WSOS, then \( q_\nu \neq 0 \) and there exist operators and a state on some Hilbert space that achieve winning probability \( \nu \). The proof proceeds in two stages. We first use the Hahn-Banach theorem to show (nonconstructively) the existence of a linear function that separates \( q_\nu \) from the convex cone \( \mathcal{C}_P \) and then use a GNS construction, as described below. Unfortunately we will not in general end up with operators on a finite-dimensional Hilbert space.

We start by establishing some simple facts about \( \mathcal{C}_P \).

**Lemma B.2.** Let \( W \) be the product of some number of variables from the set \( \{X_{s_i}^{a_j}\} \). Then \( \mathbb{I} - W^\dagger W \in \mathcal{C}_P \), and \( \mathbb{I} - WW^\dagger \in \mathcal{C}_P \).
Proof. The proof is by induction on $n$, the number of variables in the product $W$. For $n = 1$, we have to show that for all $j, a_j, s_j, \| - (X_{s_j}^{a_j})^2 \| \in C_P$. We do this for $\| - (X_{s_j}^{a_j})^2 \|$.

Writing

$$\| - (X_{s_j}^{a_j})^2 \| = \sum_{a_j' \neq a_j} (X_{s_j}^{a_j'})^2 - \sum_{a_j} \left[(X_{s_j}^{a_j})^2 - X_{s_j}^{a_j'}\right] + \left[\| - \sum_{a_j} X_{s_j}^{a_j}\right];$$

makes it clear that $\| - (X_{s_j}^{a_j})^2 \| \in C_P$. For $n \geq 1$, write $W = VX_{s_j}^{a_j}$, where we have assumed without loss of generality that the element $X_{s_j}^{a_j}$ is rightmost in $W$, and where $V$ is the product of $n - 1$ variables. Then

$$\| - W^\dagger W \| = \| - X_{s_j}^{a_j} V^\dagger V X_{s_j}^{a_j} \| = \| - (X_{s_j}^{a_j})^2 + X_{s_j}^{a_j} (\| - V^\dagger V \|)X_{s_j}^{a_j}. $$

Now $\| - (X_{s_j}^{a_j})^2 \| \in C_P$ by the result for $n = 1$ and $\| - V^\dagger V \| \in C_P$ by the inductive hypothesis. Moreover, for any polynomial $r \in C_P$, and any arbitrary polynomial $s$, it is easy to see that $s^\dagger r s \in C_P$. Hence, this implies that $\| - W^\dagger W \| \in C_P$. The argument for $\| - W W^\dagger \|$ is analogous. 

Lemma B.3. Let $p$ be a Hermitian polynomial. Then there exists a real number $t \geq 0$ and an $s \in C_P$ such that $p = s - t \|$. 

Proof. The polynomial $p$ is a finite sum of terms of the form $p' = w^* v W^\dagger V + w v^* V^\dagger W$, where $V, W$ are products of the variables, $w, v \in C$ and $w^*$ is the complex conjugate of $w$ (likewise for $v^*$). If we can show the result for $p'$, then the result for general polynomials $p$ follows immediately. To this end, note that we can write

$$p' = (v^* V^\dagger + w^* W^\dagger)(v V + w W) - |v|^2 V^\dagger V - |w|^2 W^\dagger W$$

so that

$$| |v|^2 + |w|^2 | \| + p' = (v^* V^\dagger + w^* W^\dagger)(v V + w W) + |v|^2 (\| - V^\dagger V) + |w|^2 (\| - W^\dagger W)$$

which is in $C_P$ by Lemma B.2. Taking $t = |v|^2 + |w|^2$, the result follows for $p'$, which in turn implies the result for general polynomials $p$. 

We now want to show that if $q$, is a Hermitian polynomial that does not lie in $C_P$, then there exists a linear functional that separates it from $C_P$. The following Lemma closely follows Proposition 3.3] where the only difference is that we consider polynomials over complex matrices instead of real Hermitian matrices. Fortunately, the essential ingredient of the proof, the Hahn-Banach theorem also holds in this case. We state entire proof for convenience:

Lemma B.4. Let $M$ be the space of Hermitian polynomials over complex matrices. Let $q$ be a Hermitian polynomial such that $q \notin C_P$. Then there exists a linear functional $\lambda : M \rightarrow \mathbb{R}$ such that $\lambda(C_P) \geq 0, \lambda(\|) > 0, \lambda(q) \leq 0$.

Proof. Let $M$ be the space of Hermitian polynomials over complex matrices. Let $\mu : M \rightarrow \mathbb{R}$ be a linear functional defined as $\mu(p) := \inf \{ t > 0 : p = s - t \| \text{ for some } s \in C_P \}$. Note that by Lemma B.3, we can express any $p \in M$ in this form. Clearly, $\mu$ is a seminorm on $M$. Note that for $q \notin C_P$ we have $\mu(q - \|) \geq 1$ by definition. We consider now a fixed $q \notin C_P$ and let $L$ be the span of $q - \|$ in $M$, i.e., all Hermitian polynomials $t(q - \|)$ with $t \in \mathbb{R}$. Define a linear functional $f : L \rightarrow \mathbb{R}$ so that $f(t(q - \|)) := t$. It is not hard to see that $f \leq \mu$ on $L$. Now we make the
first nonconstructive step. By the Hahn-Banach theorem \([44], \text{Theorem 3.3}\), \(f\) extends to a linear functional \(F : M \rightarrow \mathbb{R}\) such that \(F(p) \leq \mu(p)\) for all \(p \in M\).

We now claim that \(\lambda = -F\) satisfies the requirements of the lemma: First of all, note that we have for all \(s \in \mathcal{C}_P\) that \(F(s) - F(q) + 1 = F(s - q + (q - I)) = F(s - I) \leq \mu(s - I) \leq 1\), where the first equality follows from the linearity of \(F\), and the first inequality follows from \(F\) being an extension of \(f\). Hence, \(F(s) \leq F(q)\). Clearly, we also have that for all \(s \in \mathcal{C}_P\) and \(t > 0\), \(ts \in \mathcal{C}_P\) and hence \(tF(s) = F(ts) \leq F(q)\). Thus, if \(s \in \mathcal{C}_P\) then \(F(s) \leq 0\) and \(F(q) \geq 0\). Hence, \(\lambda = -F\) satisfies \(\lambda(\mathcal{C}_P) \geq 0\) and \(\lambda(q) \leq 0\) as required.

It remains to show that \(\lambda(\mathbb{I}) > 0\). First of all, note that \(\mathbb{I} \in \mathcal{C}_P\). Suppose that on the contrary we have \(\lambda(\mathbb{I}) = 0\). Let \(p \in \mathcal{C}_P\) and note that by Lemma \([3.3]\) we may write \(-p = s - t\mathbb{I}\) for some \(t > 0\) and \(s \in \mathcal{C}_P\). From \(t\mathbb{I} = s + p\), we have \(0 = t\lambda(\mathbb{I}) = \lambda(t\mathbb{I}) = \lambda(s) + \lambda(p) \geq 0\) and hence \(\lambda(s) = \lambda(p) = 0\) for all \(p \in \mathcal{C}_P\). Now note that since \(\mathbb{I} - q \in M\) we may write \(\mathbb{I} - q = r - s\) for some \(r, s \in \mathcal{C}_P\). But then \(0 = \lambda(r) - \lambda(s) = \lambda(\mathbb{I} - q) = 1\) which is a contradiction. \(\square\)

The remainder of the proof of Theorem 5.2 is now exactly identical to \([23]\), which in itself is analogous to the famous GNS construction \([46, 7]\) that allows us to find a representation in terms of bounded operators on a Hilbert space. We here provide a slightly annotated version of this approach in the hope that it will be more accessible to the present audience.

**Theorem B.5** (Helton and McCullough). Let \(M\) be the space of Hermitian polynomials. Let \(\lambda : M \rightarrow \mathbb{R}\) be a linear functional such that \(\lambda(\mathcal{C}_P) \geq 0\) and \(\lambda(\mathbb{I}) > 0\). Then there exists a Hilbert space \(\mathcal{H}\), bounded operators \(\{\hat{X}^{a_j}_s\}\) on \(\mathcal{H}\), and a state \(\gamma \in \mathcal{H}\) such that for all \(p \in \mathcal{P}\) we have \(\lambda(\{\hat{X}^{a_j}_s\}) \geq 0\) and for any Hermitian \(q \in M\),

\[
\langle \gamma | q(\{\hat{X}^{a_j}_s\}) | \gamma \rangle = \lambda(q).
\]

**Proof.** First, we construct a Hilbert space \(\mathcal{H}\) from \(M\): For \(s, t \in M\), define

\[
\langle s | t \rangle = \frac{1}{2} \lambda(s^\dagger t + t^\dagger s).
\]

It is easy to verify that \(\langle s | t \rangle\) is symmetric, bilinear and is also positive semidefinite whenever \(s = t\), since \(s^\dagger s \in \mathcal{C}_P\) and hence \(\langle s | s \rangle = \lambda(s^\dagger s) \geq 0\). Note that \(\langle \cdot | \cdot \rangle\) is degenerate, but in order to obtain a Hilbert space, we need to turn \(\langle \cdot | \cdot \rangle\) into an inner product. This can be done in the standard way by 'moding out' the degeneracy: Consider

\[
\mathcal{J} = \{s \in M \mid \langle s | s \rangle = 0\}.
\]

It is not difficult to verify that \(\mathcal{J}\) forms a linear subspace of \(M\) and that \(\mathcal{J}\) is a left ideal of \(M\) We now consider the quotient space \(M/\mathcal{J}\), which is the vector space created by the equivalence classes

\[
[x] = \{x + j \mid j \in \mathcal{J}\}.
\]

Addition and scalar multiplication are defined via the following operations inherited from \(M\): for \(x, y \in M\) and \(\alpha \in \mathbb{C}\), we have \([x + y] = [x] + [y]\) and \([\alpha x] = \alpha[x]\). We can now define the inner product

\[
\langle [x] | [y] \rangle = \langle x | y \rangle.
\]
It is important to note that this inner product does not depend on our choice of representative from each equivalence class, and we have eliminated the degeneracy present earlier. The Hilbert space is now obtained by forming the completion of \( M/\mathcal{J} \) with respect to this inner product.

Second, we now need to show that there exists a representation \( \pi : M \to \mathbb{B}(\mathcal{H}) \). We first define the action of \( \pi(x) \) with \( x \in M \) on the vectors \([y]\) as

\[
X[y] = [xy],
\]

where we use the shorthand \( X = \pi(x) \). It is straightforward to verify that this definition is again independent of our choice of representative from each equivalence class, and that \( \pi \) is a homomorphism. For simplicity, we only show boundedness for operators \( \{X_{s_j}^a\} \in M \). To see that \( X = \pi(x) \) for \( x \in \{X_{s_j}^a\} \) is bounded, note that by Lemma \[B.2\] we have \( \mathbb{I} - x^\dagger x \in \mathcal{C}_\mathcal{P} \) and that

\[
\langle X[s] | X[s] \rangle = \langle xs | xs \rangle = \langle s | s \rangle - \lambda(s^\dagger (\mathbb{I} - x^\dagger x)s),
\]

where \( \lambda(s^\dagger (\mathbb{I} - x^\dagger x)s) \geq 0 \), since \( s^\dagger (\mathbb{I} - x^\dagger x)s \in \mathcal{C}_\mathcal{P} \). From Lemma \[B.2\] we also have that \( \mathbb{I} - xx^\dagger \in \mathcal{C}_\mathcal{P} \), and hence the argument for \( \pi(x^\dagger) \) is analogous and we may write \( X^\dagger = \pi(x^\dagger) \) without ambiguity. Hence we can find claimed operators \( \{\tilde{X}_{s_j}^a\} \in \mathbb{B}(\mathcal{H}) \).

Third, we need to define the vector \( \gamma \). Since \( \mathbb{I} \in M \) we choose \( \gamma = [\mathbb{I}] \). Hence, \( \langle \gamma | \gamma \rangle = \lambda(\mathbb{I}) > 0 \), and thus \( \gamma \) is non-zero. Let \( q \in M \) and write \( q(X) \) for the polynomial where variables \( x_j \) have been substituted by their representations \( X_j \). Note that

\[
\langle q(X)\gamma | \gamma \rangle = \lambda(q),
\]

where we have used the fact that \( q \) is a Hermitian polynomial. By a similar argument, it follows that for \( p \in \mathcal{C}_\mathcal{P} \) and \( r \in M \) we have

\[
\langle p(X)[r] | [r] \rangle = \lambda(r^\dagger pr) \geq 0,
\]

since \( r^\dagger pr \in \mathcal{C}_\mathcal{P} \) and hence \( p(X) \geq 0 \) as promised. \( \square \)

We can now complete the proof of Theorem \[4.3\]

**Proof of Theorem \[4.3\]** Recall that our goal was to prove the contrapositive: If \( q_\nu \notin \mathcal{C}_\mathcal{P} \) then \( q_\nu \neq 0 \). From Lemma \[B.4\] we have that if \( q_\nu \notin \mathcal{C}_\mathcal{P} \), then there exists a linear functional \( \lambda \) that separates \( q_\nu \) from \( \mathcal{C}_\mathcal{P} \). Lemma \[B.5\] gives us that there exists a Hilbert space \( \mathcal{H} \), measurement operators \( \{\tilde{X}_{s_j}^a\} \), and a vector \( \gamma \) such that

\[
\lambda(q_\nu) = \langle \gamma | q_\nu(\{\tilde{X}_{s_j}^a\}) | \gamma \rangle \leq 0.
\]

and the operators satisfy all the constraints, i.e., for all \( p \in \mathcal{P} \) we have \( p(\{\tilde{X}_{s_j}^a\}) \geq 0 \). (Note that we only have equality constraints, which we implemented by including both \( p \) and \(-p \) in \( \mathcal{P} \).) Since \( \gamma \) is not zero, we have \( q_\nu \neq 0 \) which completes the proof. \( \square \)

Unfortunately, Theorem \[B.5\] does not tell us whether the underlying Hilbert space \( \mathcal{H} \) is finite-dimensional, or whether the algebra generated by the operators \( \{\tilde{X}_{s_j}^a\} \) is type-I at all. Hence, we cannot ensure without further proof that the fact that our measurement operators do satisfy the commutation constraints necessarily leads to them having tensor product form. Thus, we do not know whether there exist games \( G \) for which \( \omega^*(G) < \omega^f(G) \): for such games we may would have to get a type-II or type-III algebra.
C Tool 3: Semidefinite Programming

A semidefinite program (SDP) is an optimization over Hermitian matrices \( [47] \). The objective function depends linearly on the matrix variable and the optimization is carried out subjected to the matrix variable being positive semidefinite and satisfies various affine constraints. Any semidefinite program may be written in the following standard form \( [6] \):

\[
\begin{align*}
\text{maximize} & \quad - \text{Tr} \left[ G_0 Z \right], \\
\text{subject to} & \quad \text{Tr} \left[ G_k Z \right] = b_k \quad \forall k, \\
& \quad Z \geq 0,
\end{align*}
\]

(32a) \hspace{1cm} (32b) \hspace{1cm} (32c)

where \( G_0 \) and all the \( G_k \)'s are Hermitian matrices, and the \( b_k \) are real numbers that together specify the optimization; \( Z \) is the Hermitian matrix variable to be optimized.

An SDP also arises in the inequality form, which seeks to minimize a linear function of the optimization variables \( (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n \), subjected to a linear matrix inequality:

\[
\begin{align*}
\text{minimize} & \quad b_k^\prime x_k \\
\text{subject to} & \quad F_0 + \sum_{k=1}^{6} x_k F_k \geq 0.
\end{align*}
\]

(33a) \hspace{1cm} (33b)

As in the standard form, \( F_0 \) and all the \( F_k \)'s are Hermitian matrices, while \( (b_1^\prime, b_2^\prime, \ldots, b_n^\prime) \) is a real vector of length \( n \).

D Some Other Miscellaneous Details

D.1 Implementing Lowest Level SDP Relaxations for \( I_{3322} \)

Here, we will provide the explicit form for the matrices \( F_k \) and constants \( b_k^\prime \) that define the SDP used in the lowest level relaxation for finding an upper bound on \( \omega^* (I_{3322}) \). Note that as with the CHSH case, in the lowest level relaxation, we shall choose \( s_{ij} \) in Eq. (8) as multiples of \( \mathbb{I} \). To this end, we will write the SDP in the inequality form as

\[
\begin{align*}
\text{minimize} & \quad b_\nu^\prime \nu + \sum_{k=1}^{6} b_k^\prime x_k \\
\text{subject to} & \quad \Gamma = F_0 + \nu F_\nu + \sum_{k=1}^{6} x_k F_k \geq 0.
\end{align*}
\]

(34a) \hspace{1cm} (34b)

In particular, we will set

\[
F_0 = \frac{1}{27} \begin{pmatrix}
0 & 1 & 0 & 0 & 2 & 1 & 0 \\
1 & 0 & 0 & 0 & -1 & -1 & -1 \\
0 & 0 & 0 & 0 & -1 & -1 & 1 \\
0 & 0 & 0 & 0 & -1 & 1 & 0 \\
2 & -1 & -1 & -1 & 0 & 0 & 0 \\
1 & -1 & -1 & 1 & 0 & 0 & 0 \\
0 & -1 & 1 & 0 & 0 & 0 & 0
\end{pmatrix}, \quad F_\nu = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix},
\]

30
and for \( k = 1, 2, \ldots, 6 \), we shall choose \( F_k \) such that its only nonzero entries are \( [F_k]_{1,k+1} = [F_k]_{k+1,1} = 1/2 \) and \( [F_k]_{k,k+1,k+1} = -1 \). Correspondingly, \( b'_k \) is chosen such that \( b'_1 = 1 \) and \( b'_k = 0 \) for \( k = 1, 2, \ldots, 6 \). With this choice of \( F_k, b'_k \) and with \( z \) given by Eq. (17), it is easy to see that the matrix inequality constraint, Eq. (34b), ensures that

\[
 z^\dagger \Gamma z = z^\dagger \left( F_0 + \nu F_\nu + \sum_{k=1}^{6} x_k F_k \right) z = -B_{3322} - \nu \mathbb{I} + \sum_{k=1}^{6} x_k p_k = \text{SOS}
\]

where \( p_k \)'s are defined in Eq. (19) and the last equality follows from the positive semidefiniteness of \( \Gamma \).

### D.2 Implementing Higher Level SDP Relaxations for \( I_{3322} \)

In what follows, we will give a sketch of how the level 2 relaxation for \( I_{3322} \) inequality with \( z \) given by Eq. (20) can be implemented as an SDP in the inequality form, Eq. (33). Specifically, we want to write Eq. (16) as:

\[
\begin{align*}
\text{minimize} & \quad \nu, \\
\text{subject to} & \quad F_0 + \nu F_\nu + \sum_{k} x_k F_k \geq 0,
\end{align*}
\]

where, as with the lowest level relaxation, \( F_0 \) and \( F_\nu \) are real and symmetric matrices chosen such that

\[
 z^\dagger F_0 z = -B_{3322}, \quad z^\dagger F_\nu z = \mathbb{I}.
\]

Hereafter, we will focus on writing the second sum in Eq. (33) as \( \sum_k x_k z^\dagger F_k z \) for some appropriate choice of Hermitian matrix \( F_k \) where \( x_k \) is some variable to be optimized. As opposed to the lowest level relaxation, the most general second level relaxation would require that each \( s_{ij} \) in Eq. (33) is a polynomial of degree at most 1. Let \( s_{ij} = \sum_k \lambda_{ijk} M_k \) where \( M_k \) is the \( k \)-entry of the vector \( \mu = (I, A_1^a, A_2^a, A_3^a, B_1^b, B_2^b, B_3^b) \) which consists of all degree 1 or lower monomials that can be found in \( z \). For a fixed \( i \) and \( j \), we thus have

\[
 s_{ij}^\dagger p_i s_{ij} = \sum_{k,l} M_k^\dagger \left( \lambda_{ijk}^* \lambda_{ijl} \right) p_i M_l = \mu^\dagger \Lambda_{ij} p_i \mu,
\]

where here \( \lambda_{ijk}^* \) is the complex conjugate of \( \lambda_{ijk} \), \( p_i \mu \) is a vector formed by multiplying each entry of \( \mu \) by \( p_i \) and \( \Lambda_{ij} \) is a \( 7 \times 7 \) matrix with its \((k,l)\)-entry given by \( \lambda_{ijk}^* \lambda_{ijl} \). Clearly, as it is, \( \Lambda_{ij} \) is a rank 1 but otherwise arbitrary positive semidefinite matrix. Analogously, we see that if we further perform a sum over \( j \) in Eq. (37), then we may write \( \sum_j s_{ij}^\dagger p_i s_{ij} = \mu^\dagger \Lambda_i p_i \mu \) where \( \Lambda_i = \sum_j \Lambda_{ij} \) is now an arbitrary positive semidefinite matrix. Moreover, the requirement of \( \Lambda_i \) being positive semidefinite can also be removed if we recall the fact that in the case of \( I_{3322} \) inequality, if \( p_i \) is in \( \mathcal{P} \), so is \(-p_i \). Then, what remains to be done is to express \( \sum_j s_{ij}^\dagger p_i s_{ij} \) and hence \( \mu^\dagger \Lambda_i p_i \mu \) in the form \( z^\dagger \Omega_i z \) for some Hermitian \( \Omega_i \). Evidently, the entries in \( \Lambda_i \) will be related to the entries in \( \Omega_i \) linearly. For example, since

\[
\begin{align*}
[A_1]_{6,5} M_4^\dagger p_1 M_5 = & [A_1]_{6,5} (B_2^b)^\dagger \left[ (A_1^a)^2 - (A_1^a) \right] (B_2^b) \\
= & [A_1]_{6,5} \left[ (A_1^a B_2^b)^\dagger (A_1^a B_2^b) - (B_2^b)^\dagger (A_1^a B_2^b) \right],
\end{align*}
\]

31
we may make the following identification $[\Omega_1]_{9,8} = -[\Omega_1]_{8,8} = [\Lambda_1]_{6,5}$ and so on. Each independent entry of $\Lambda_i$ therefore corresponds to an independent optimization variable $x_k$ and some Hermitian matrix $F_k$ via $\Omega_i$. In the example above, the $F_k$ corresponding to (the real part of) $[\Lambda_1]_{6,5}$ would be zero everywhere except for its $(6,8)$, $(9,8)$, $(8,6)$ and $(8,9)$ entry, which reads as $-1,1,-1,1$ respectively. More intuitively, each of these $F_k$’s gives rise to some polynomial identities such that $z^\dagger F_k z = 0$ whenever the constraints are satisfied. Putting everything together, we see that the search for a positive semidefinite $\Gamma$ such that

$$\nu \| - B_{3322} - \sum_k x_k z^\dagger F_k z = z^\dagger \Gamma z,$$

for some appropriate choice of $F_k$. Comparing this with Eq. (35) and Eq. (36), we see that evidently any higher order relaxation in our hierarchy can also be implemented as an SDP.

### D.3 Yao’s inequality

Here, we note that for $\{A_i, B_j, C_k\}_{i,j,k=1,2,3}$ satisfying the commutation relations $[A_i, B_j] = 0$, $[A_i, C_k] = 0$, $[B_j, C_k] = 0$ and for $\Gamma$ given by Eq. (25), we have

$$3\sqrt{3} \| - B_{Yao} = z^\dagger \Gamma z + \sum_{i,j,k} \alpha_{ijk} \left( \| - t_{ijk}^\dagger t_{ijk} \right) + \frac{1}{2\sqrt{3}} \sum_{i,j,k} \sum_{l=A,B,C} \left( f_{ijk}^{(A)} + f_{ijk}^{(B)} + f_{ijk}^{(C)} + f_{ijk}^{(A)^\dagger} + f_{ijk}^{(B)^\dagger} + f_{ijk}^{(C)^\dagger} \right),$$

where $t_{ijk} := A_i B_j C_k$,

$$\alpha_{ijk} = \begin{cases} \frac{1}{2\sqrt{3}} & : i \neq j \neq k, \\ 0 & : i = j = k, \\ \frac{1}{12\sqrt{3}} & : \text{otherwise}. \end{cases}$$

and the second sum $\sum_{l=A,B,C}$ is over all possible $i, j, k$ such that $i \neq j \neq k$. In contrast with Eq. (26), the above equality holds even if none of the constraints $A_i^2 = B_j^2 = C_k^2 = \|$ are satisfied. Moreover, the above equality can also be cast in the form of Eq. (8) with the help of identities such as

$$\| - t_{ijk}^\dagger t_{ijk} = p_k^{(C)} + C_k^\dagger p_j^{(B)} C_k + g_{jk} p_k^{(A)} g_{jk},$$

and

$$f_{ijk}^{(A)} + f_{ijk}^{(A)^\dagger} = 2g_{jk} p_i^{(A)} g_{jk} + 2g_{kj} p_i^{(A)} g_{kj} - g_{jk} \left( p_j^{(A)} + p_k^{(A)} \right) g_{jk} - g_{kj} \left( p_j^{(A)} + p_k^{(A)} \right) g_{kj}$$

$$+ (g_{jk} + g_{kj})^\dagger p_j^{(A)} (g_{jk} + g_{kj}) + (g_{jk} + g_{kj})^\dagger p_k^{(A)} (g_{jk} + g_{kj})$$

$$- 2 (g_{jk} + g_{kj})^\dagger p_i^{(A)} (g_{jk} + g_{kj}),$$

where $g_{jk} := B_j C_k$. 

32