

Causal Compatibility Inequalities Admitting of Quantum Violations in the Triangle Scenario

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Quantum correlations are often incompatible with a classical assumption of causal structure. This nonclassicality is often known as quantum nonlocality, and it is witnessed through the violation of causal compatibility inequalities, such as Bell inequalities. Such inequalities were recently derived for the Triangle scenario [arXiv:1609.00672], begging the question: can these inequalities be violated by quantum correlations? Here we answer this affirmatively, and discuss specific Triangle scenario inequalities and quantum configurations which manifest nonclassical correlations. Numerical optimizations reveal quantum resources potentially qualitatively different from those known previously.

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I. INTRODUCTION

- Todo (TC Fraser): Overview of importance of inequalities
- Todo (TC Fraser): Triangle Scenario and existing work
- Todo (TC Fraser): Objective of research project
- Todo (TC Fraser): Structure of this paper

II. CAUSAL COMPATIBILITY

- Todo (TC Fraser): Define marginal scenario
- Todo (TC Fraser): Define marginal model
- Todo (TC Fraser): Define causal structure
- Todo (TC Fraser): Define compatibility

III. TRIANGLE SCENARIO

- Todo (TC Fraser): Discuss some of its appearances in other work
- Todo (TC Fraser): Figure

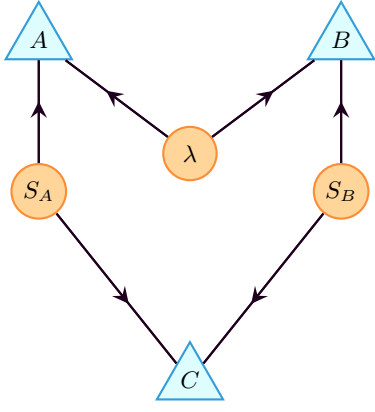


FIG. 1. The triangle scenario re-imagined to mimic the Bell scenario. The measurement settings S_A, S_B are latent nodes unlike the Bell scenario (fig. 2).

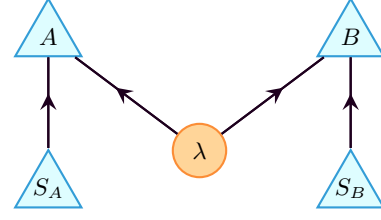


FIG. 2. The Bell scenario consisting of two observers A, B together with measurement settings S_A and S_B respectively.

A. Fritz Distribution

As was originally noticed by Fritz [1], it is possible to construct quantum distributions incompatible with the triangle scenario by utilizing quantum distributions incompatible with the familiar Bell scenario. To explain, imagine rearranging the triangle into the configuration depicted in fig. 1 and contrast it with the Bell scenario of fig. 2. The crucial distinction to be made is that the respective measurement settings S_A, S_B in the Bell scenario become latent nodes in the triangle scenario. In order to embed Bell scenario incompatibility into the triangle scenario, the latent nodes S_A, S_B need to be observable and independent of the shared latent node λ . This can be accomplished by having C measure the measurement settings S_A, S_B and announce them as an outcome. Consequently, any distribution over A, B, S_A, S_B that is incompatible with Bell scenario is also incompatible with the triangle scenario provided that C is perfectly correlated with S_A, S_B . Understandably there are numerous ways that this can be accomplished, albeit we will focus on elucidating an exemplary case.

The **Fritz distribution**, denoted P_F , is a quantum-accessible distribution known to be incompatible with the triangle scenario [1]. Explicitly, the Fritz distribution can be written as follows:

$$\begin{aligned} P_F(000) &= P_F(110) = P_F(021) = P_F(131) = P_F(202) = P_F(312) = P_F(233) = P_F(323) = \frac{1}{32}(2 + \sqrt{2}) \\ P_F(010) &= P_F(100) = P_F(031) = P_F(121) = P_F(212) = P_F(302) = P_F(223) = P_F(333) = \frac{1}{32}(2 - \sqrt{2}) \end{aligned} \quad (1)$$

Here the notation $P_F(abc) = P_{ABC}(abc) = P(A = a, B = b, C = c)$ is used as shorthand. The Fritz distribution is best visualized as a $4 \times 4 \times 4$ grid of possible outcomes as depicted in fig. 3. From this diagram, it can be seen that each of C 's outcomes restricts the possible outcomes for A, B into a 2×2 block. If one writes the outcome labels $\{0, 1, 2, 3\}$ in binary $\{00, 01, 10, 11\}$, it can be seen that the left-hand bits for A and B (respectively denoted A_l, B_l) are fixed by the outcome of C . Pursuant to the embedding of fig. 1 the left-hand bits emulate the measurement settings S_A and S_B and the right-hand bits emulate a two-outcome measurement performed by A, B as they would in fig. 2. Specifically, C 's bits are perfectly correlated with the left-bits of A, B ; $C_l = A_l$ and $C_r = B_l$. Consequently, it is possible to define the correlation between right-bits of A and B ,

$$\langle A_r B_r \rangle = P_{A_r B_r}(00) + P_{A_r B_r}(11) - P_{A_r B_r}(01) - P_{A_r B_r}(10)$$

And also define a CHSH inequality [2] for the right-bits of A and B ,

$$\langle A_r B_r | C = 00 \rangle + \langle A_r B_r | C = 01 \rangle + \langle A_r B_r | C = 10 \rangle - \langle A_r B_r | C = 11 \rangle \leq 2 \quad (2)$$

Substitution of eq. (1) into eq. (2) yields maximal violation [3],

$$3\left(\frac{1}{\sqrt{2}}\right) - \left(-\frac{1}{\sqrt{2}}\right) = 2\sqrt{2} \not\leq 2$$

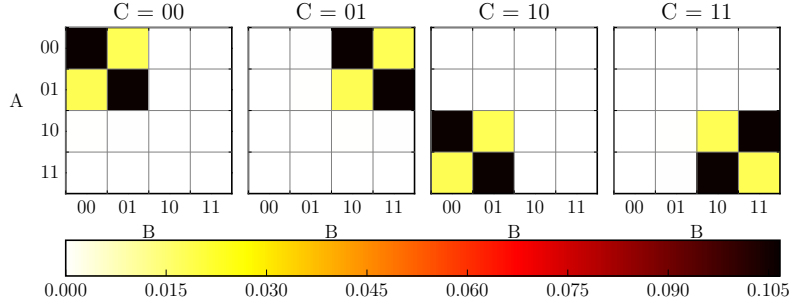


FIG. 3. The Fritz distribution visualized using a $4 \times 4 \times 4$ grid. The 4 outcomes of A, B, C are written in binary as a doublet of bits to illustrate that certain bits act as measurement pseudo-settings.

The Fritz distribution P_F can be realized as a set of quantum states and measurements. The shared resource between A and B (graphically denoted λ) is the maximally entangled Bell state:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \quad \rho_{AB} = |\Phi^+\rangle\langle\Phi^+|$$

While the states shared with C are the following mixed states:

$$\rho_{BC} = \rho_{CA} = \frac{|00\rangle\langle 00| + |11\rangle\langle 11|}{2}$$

The measurements employed by A, B and C are separable, projective measurements,

$$\begin{aligned} M_A &= \{|0\psi_1\rangle\langle 0\psi_1|, |0\psi_5\rangle\langle 0\psi_5|, |1\psi_3\rangle\langle 1\psi_3|, |1\psi_7\rangle\langle 1\psi_7|\} \\ M_B &= \{|\psi_6 0\rangle\langle \psi_6 0|, |\psi_2 0\rangle\langle \psi_2 0|, |\psi_0 1\rangle\langle \psi_0 1|, |\psi_4 1\rangle\langle \psi_4 1|\} \\ M_C &= \{|00\rangle\langle 00|, |10\rangle\langle 10|, |01\rangle\langle 01|, |11\rangle\langle 11|\} \end{aligned}$$

Where $|\psi_n\rangle$ is shorthand for,

$$|\psi_n\rangle = \frac{1}{\sqrt{2}}(|0\rangle + e^{in/4}|1\rangle)$$

Before continuing it is worth noting that eq. (1) is non-unique. Any distribution that is equal to eq. (1) via a permutation of outcomes or exchange of parties should also be referred to as a Fritz distribution. Moreover, the quantum realization presented here is not unique either. Nonetheless for concreteness, eq. (1) is taken as *the* Fritz distribution throughout this paper.

Additionally, it is important to understand the domain in which Fritz's proof of incompatibility is valid. Specifically, eq. (2) can only be applied to the triangle scenario where there exists perfect correlation between C 's outcomes and the measurement pseudo-settings (left-bits) of A and B . The details of this restriction are discussed and proven in Fritz's original work [1]. As such, the incompatibility proof employed by Fritz is not applicable to any distribution that significantly deviates from the Fritz distribution presented above. For example, if one affinely combines eq. (1) with uniform noise, at what point does the resultant distribution become compatible? This problem is discussed more in section VII.

Upon reflection, the Fritz distribution can rightly be considered slightly manufactured. The phenomenology associated with Bell non-locality or Bell incompatibility are well understood; examining these distributions under a triangle scenario embedding offers no additional perspective onto the types of resources made accessible by quantum mechanics. Therefore, it is desirable to find incompatible quantum distributions that are qualitatively different than those previously considered for the Bell scenario. In [1], Fritz presented the following problem: *Find an example of non-classical quantum correlations in the triangle scenario together with a proof of its non-classicality which does not hinge on Bell's Theorem.*¹ The problem is understandably stated ambiguously as it is not yet entirely clear how to distinguish between non-classical distributions on differing causal structures. To refine the discussions, consider the following refinements of the problem:

¹ In the way Fritz defines, *non-classical* correlations are the class of *incompatible* correlations.

1. Find proofs of causal incompatibility of quantum distributions on the triangle scenario that are not reliant on perfect correlations.
2. Find incompatible quantum distributions on the triangle scenario that are *more incompatible* than all Fritz-type embeddings.

Todo (TC Fraser): Discuss the accomplishments of this paper towards answering these problems.

IV. INFLATION TECHNIQUE

- Todo (TC Fraser): Summarize inflation technique
- Todo (TC Fraser): Inflations of Triangle Scenario
- Todo (TC Fraser): Demonstrate that one can derive causal incompatibility inequalities from inflation
- Todo (TC Fraser): Pre-injectable sets for Large inflation

V. DERIVING INEQUALITIES

- Todo (TC Fraser): Marginal problem
- Todo (TC Fraser): Popular methods: Fourier Motzkin (Convex hull, Polytope projection), Hardy implication inequalities, linear program/certificate
- Todo (TC Fraser): Overview incidence for Large Inflation
- Todo (TC Fraser): Rule out expensive methods like FM
- Todo (TC Fraser): Present some of the inequalities found

A. Symmetric Inequalities

- Todo (TC Fraser): Discuss symmetries and why they are useful
- Todo (TC Fraser): Symmetrizing Incidence Matrix
- Todo (TC Fraser): Large inflation incidence contracted drastically
- Todo (TC Fraser): Present some of the inequalities found

VI. VIOLATIONS

- Todo (TC Fraser): Fritz Distribution violates found inequalities

A. Numerical Optimizations

- Todo (TC Fraser): Generic idea
- Todo (TC Fraser): Optimization techniques used

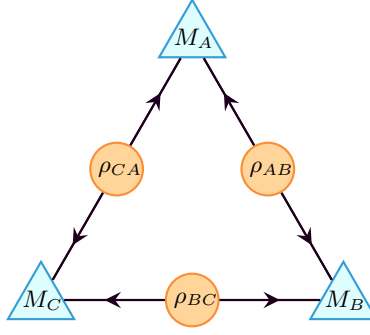


FIG. 4. The triangle scenario as modeled by quantum states and measurements.

B. Parameterizing Quantum Distributions

In search of new, incompatible, quantum distributions that can be realized on the triangle scenario, numerical optimizations over the space of quantum-accessible probability distributions are performed. To do so, we are interested in a parameterization all distributions that can be expressed as follows:

$$P_{ABC}(abc) = \text{Tr}[\Pi^\top \rho_{AB} \otimes \rho_{BC} \otimes \rho_{CA} \Pi M_{A,a} \otimes M_{B,b} \otimes M_{C,c}] \quad (3)$$

Where $\rho_{AB}, \rho_{BC}, \rho_{CA}$ are bipartite density matrices, M_A, M_B, M_C are generic measurements sets and Π is a permutation matrix that aligns the states and measurements appropriately².

In order to qualify the scope of eq. (3) and associated computational complexity of the parameterization, there are two restrictions that are made with justification. The states ρ are taken to be bipartite *qubit* states acting on $\mathcal{H}^2 \otimes \mathcal{H}^2$. This is motivated by section III A in which the Fritz distribution only requires qubit states. In generality, one could consider n -dimensional states acting on $\mathcal{H}^n \otimes \mathcal{H}^n$. However, in such cases the joint density matrix $\rho_{AB} \otimes \rho_{BC} \otimes \rho_{CA}$ then acts on $(\mathcal{H}^n)^{\otimes 6}$ requiring a $n^6 \times n^6$ matrix with n^{12} entries. Therefore, $n = 2$ is far more computationally feasible than $n > 2$. Additionally, restrict our focus to projective-valued measures (PVMs) instead of projective-operator valued measures (POVMs) for three reasons. First, section III A demonstrates that PVMs are sufficient for witnessing incompatible quantum distributions in the triangle scenario. Second, generating k -outcome POVM measurements is possible using rejection sampling techniques [4], however a valid, unbiased parameterization was not found for $k > 2$. Finally, PVMs provide considerable computational advantage over POVMs as they permit eq. (3) to be re-written as follows:

$$P_{ABC}(abc) = \langle m_{A,a} m_{B,b} m_{C,c} | \Pi^\top \rho_{AB} \otimes \rho_{BC} \otimes \rho_{CA} \Pi | m_{A,a} m_{B,b} m_{C,c} \rangle \quad (4)$$

In order to parameterize all such distributions, we elect to parameterize the states and measurements separately. Although there are numerous techniques that can be used when parameterizing quantum states and measurements [4–9], a single technique is presented that was found to be most computationally suitable for our purposes.

1. Unitary Group

To facilitate the parameterization of quantum states and PVMs, a parameterization of the unitary group of dimension d (denoted $\mathcal{U}(d)$) by Spengler, Huber and Hiesmayr [10] is introduced. Discussions of its application to states and measurements are deferred to section VIB 3 and section VIB 2 respectively.

In Ref. [10], Spengler *et. al.* proved that all unitaries $U \in \mathcal{U}(d)$ can be parameterized without degeneracy as follows:

$$U = \left[\prod_{m=1}^{d-1} \left(\prod_{n=m+1}^d \exp(iP_n \lambda_{n,m}) \exp(i\sigma_{m,n} \lambda_{m,n}) \right) \right] \left[\prod_{l=1}^d \exp(iP_l \lambda_{l,l}) \right] \quad (5)$$

² Π is discussed more thoroughly in section VIB 4.

Where $\lambda = \{\lambda_{n,m} \mid n, m \in 1, \dots, d\}$ form a $d \times d$ matrix of real-valued parameters with periodicities $\lambda_{m,n} \in [0, \frac{\pi}{2}]$ for $m < n$ and $\lambda_{m,n} \in [0, 2\pi]$ for $m \geq n$.

$$\lambda = \begin{pmatrix} \lambda_{1,1} & \cdots & \lambda_{1,d} \\ \vdots & \ddots & \vdots \\ \lambda_{d,1} & \cdots & \lambda_{d,d} \end{pmatrix}$$

And where P_l are one-dimensional projective operators,

$$P_l = |l\rangle\langle l| \quad 1 \leq l \leq d \quad (6)$$

and the $\sigma_{m,n}$ are generalized anti-symmetric σ -matrices,

$$\sigma_{m,n} = -i|m\rangle\langle n| + i|n\rangle\langle m| \quad 1 \leq m < n \leq d$$

The SSH parameterization (eq. (5)) is unique in that each of the real-valued parameters $\lambda_{n,m}$ has physical significance. For the sake of reference, let us label the matrix exponential terms in eq. (5) in a manner that corresponds to their affect on an orthonormal basis $\{|1\rangle, \dots, |d\rangle\}$.

$$\begin{aligned} GP_l &= \exp(iP_l\lambda_{l,l}) \\ RP_{n,m} &= \exp(iP_n\lambda_{n,m}) \\ R_{m,n} &= \exp(i\sigma_{m,n}\lambda_{m,n}) \end{aligned} \quad (7)$$

For example, $R_{m,n} = \exp(i\sigma_{m,n}\lambda_{m,n})$ applies a rotation to the sub-space spanned by $|m\rangle$ and $|n\rangle$ for $m < n$. Analogously, $RP_{n,m}$ generates the relative phase between $|m\rangle$ and $|n\rangle$ for $m > n$ and GP_l fixes the global phase of $|l\rangle$. Possessing a parameterization that maintains this physical interpretation is useful as it allows one to readily eliminate any degeneracies. For the purposes of quantum distributions such as eq. (3), it should be clear that any contributions to global phase are irrelevant. The SSH parameterization becomes especially attractive because it readily permits one to drop the global phase terms by setting $\lambda_{l,l} = 0$ for all $l = 1, \dots, d$. It is convenient to denote the set of all unitaries up to global phase considerations as $\tilde{\mathcal{U}}(d)$ and express $\tilde{U} \in \tilde{\mathcal{U}}(d)$ using $d(d-1)$ real-valued parameters:

$$\tilde{U} = \prod_{m=1}^{d-1} \left(\prod_{n=m+1}^d RP_{n,m} R_{m,n} \right) \quad (8)$$

Another attractive feature of the SSH parameterization not mentioned in [10] is that eq. (5), and thus eq. (8), can be implemented in a computationally efficient manner. This is discussed in appendix A.

2. Measurements

For each measurement set M in eq. (3), we consider a d -element projective-valued measure (PVM) $M = \{M_1, \dots, M_d\}$ satisfying a number of familiar constraints:

$$\begin{aligned} \forall |\phi\rangle \in \mathcal{H}^d : \langle \phi | M_i | \phi \rangle &\geq 0 & \sum_{i=1}^d M_i &= \mathbb{1}_d \\ M_i &= |m_i\rangle\langle m_i| & M_i M_j &= \delta_{ij} M_i \end{aligned}$$

Therefore, parameterizing M corresponds to parameterizing the set of all orthonormal basis $\{|\psi_1\rangle, \dots, |\psi_d\rangle\}$ of \mathcal{H}^d . First note that any such basis can be transformed into the computational basis $\{|1\rangle, \dots, |d\rangle\}$ by a unitary denoted $U^{-1} \in \mathcal{U}(d)$.

$$\forall i : U^{-1}|\psi_i\rangle = |i\rangle \quad (9)$$

With this observation, all that is required is to parameterize the set of all unitaries $U \in \mathcal{U}(d)$. Specifically, the projective property each $M_i \in M$ means that the global phase of U is completely arbitrary; one only needs to consider parameterizing unitaries up to global phase using eq. (8).

$$M = \{\tilde{U}|i\rangle\langle i|\tilde{U}^\dagger \mid i \in \{1, \dots, d\}\}$$

For the purposes discussed in section VIB, only $d = 4$ outcome measurements are utilized and therefore requiring $4(4-1) = 12$ real-valued parameters. This method was inspired by the measurement seeding method of Pál and Vértési's [11] iterative optimization technique.

3. States

Each state $\rho \in (\rho_{AB}, \rho_{BC}, \rho_{CA})$ of eq. (3) is modeled as a two-qubit density matrices acting on $\mathcal{H}^2 \otimes \mathcal{H}^2$. The space of all such states corresponds to the space of all 4×4 positive semi-definite hermitian matrices with unitary trace.

$$\forall |\phi\rangle \in \mathcal{H}^d : \langle \phi | \rho | \phi \rangle \geq 0 \quad \rho^\dagger = \rho \quad \text{Tr}(\rho) = 1 \quad (10)$$

Although is common to parameterize all such matrices using a Cholesky decomposition [8], we make use of the non-degenerate SHH parameterization [10] and the spectral decomposition of ρ . Retaining full generality, consider full-rank density matrices:

$$\rho = \sum_{i=1}^d p_i |\psi_i\rangle \langle \psi_i| \quad \sum_{i=1}^d p_i = 1, p_i \geq 0 \quad (11)$$

Where $\{p_i\}$ are the eigenvalues of ρ and $\{|\psi_i\rangle\}$ are its eigenstates. It is here that one recognizes the reapplication of eq. (9): any orthonormal basis $\{|\psi_i\rangle\}$ of \mathcal{H}^d can be transformed into a computational basis $\{|i\rangle\}$ by a unitary transformation $U \in \mathcal{U}(d)$ such that $|\psi_i\rangle = U|i\rangle$. Analogous to the projective measurements considered in section VIB 2, the global phase contributions are redundant.

$$\rho = \sum_{i=1}^d p_i \tilde{U}|i\rangle \langle i| \tilde{U}^\dagger$$

Parameterizing the eigenvalues requires $d - 1$ real-valued parameters due to the trace constraint of eq. (10). The eigenvalues are parameterized without degeneracy using a tuple of $d - 1$ parameters $\lambda = (\lambda_1, \dots, \lambda_{d-1})$, $\lambda_i \in [0, 2\pi]$ using hyperspherical coordinates [5, 10]:

$$\begin{aligned} p_n &= \prod_{i=1}^{n-1} \sin^2 \lambda_i \\ p_j &= \cos^2 \lambda_j \prod_{i=1}^{j-1} \sin^2 \lambda_i \quad \forall j \in 1, \dots, n-1 \end{aligned} \quad (12)$$

Therefore it is possible to parametrize all d -dimensional density matrices satisfying eq. (10) using $d(d-1) + d - 1 = d^2 - 1$ parameters.

4. Permutation Matrix

Finally, we introduce the a permutation matrix Π for the triangle scenario. For bipartite qubit states, Π is the 64×64 bit-wise matrix depicted in fig. 5. Upon examination of eq. (4), we consider Π to be acting on the joint global state $\rho_{AB} \otimes \rho_{BC} \otimes \rho_{CA}$. To illuminate its necessity, consider eq. (3) in the absence of Π .

$$\begin{aligned} P_{ABC}(abc) &\stackrel{?}{=} \text{Tr}[(\rho_{AB} \otimes \rho_{BC} \otimes \rho_{CA})(M_A^a \otimes M_B^b \otimes M_C^c)] \\ &= \text{Tr}[(\rho_{AB} M_A^a) \otimes (\rho_{BC} M_B^b) \otimes (\rho_{CA} M_C^c)] \\ &= \text{Tr}(\rho_{AB} M_A^a) \text{Tr}(\rho_{BC} M_B^b) \text{Tr}(\rho_{CA} M_C^c) \\ &= P_{A|\rho_{AB}}(a) P_{B|\rho_{BC}}(b) P_{C|\rho_{CA}}(c) \end{aligned}$$

On an operational level, this corresponds to A making a measurement on *both* subsystems of ρ_{AB} and *not* on any component of ρ_{CA} . This is analogously troubling for B and C as well. To resolve this issue, the permutation matrix Π corresponds to *aligning* the underlying 6-qubit joint state ρ with the joint measurement M . To understand its effect, consider its effect on 6-qubit pure state $|q_1\rangle \otimes \dots \otimes |q_6\rangle = |q_1 q_2 q_3 q_4 q_5 q_6\rangle$ where $\forall i : |q_i\rangle \in \mathcal{H}^2$.

$$\Pi |q_1 q_2 q_3 q_4 q_5 q_6\rangle = |q_2 q_3 q_4 q_5 q_6 q_1\rangle$$

Π acts as a *partial transpose* on $(\mathcal{H}^2)^{\otimes 6}$ by shifting the underlying tensor structure one subsystem to the “left”. It is uniquely defined by its action on all 2^6 orthonormal basis elements of $(\mathcal{H}^2)^{\otimes 6}$,

$$\Pi \equiv \sum_{|q_i\rangle \in \{|0\rangle, |1\rangle\}} |q_2 q_3 q_4 q_5 q_6 q_1\rangle \langle q_1 q_2 q_3 q_4 q_5 q_6|$$

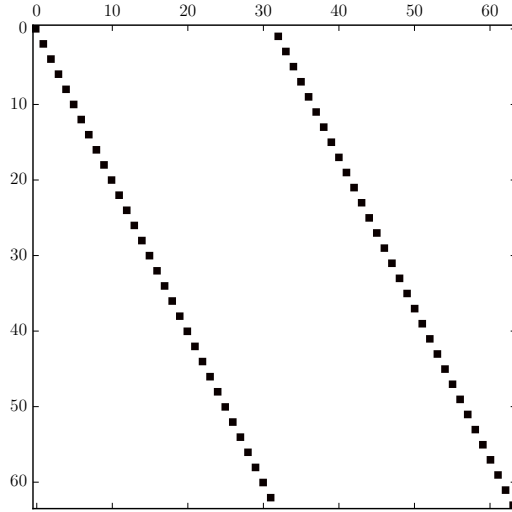


FIG. 5. The triangle scenario permutation matrix Π for $(\mathcal{H}^2)^{\otimes 6}$. Black represents a value of 1 and white represents 0.

C. Results

- Todo (TC Fraser): Plots of various optimizations
- Todo (TC Fraser): Features of maximally violating distributions

VII. NOISE

- Todo (TC Fraser): Recall why noise is important (experimental and foundational)
- Todo (TC Fraser): Describe our noise model
- Todo (TC Fraser): Plots
- Todo (TC Fraser): Define and discuss the crossing point
- Todo (TC Fraser): Discussion as to what noise measures

VIII. CONCLUSIONS

- Todo (TC Fraser): Inflation technique capable of finding inequalities witnessing quantum/classic difference in TS
- Todo (TC Fraser): Causal incompatibility inequalities found violated by known distributions
- Todo (TC Fraser): Maximal distributions are different than Fritz but still rely on Bell's theorem
- Todo (TC Fraser): Refinement on Fritz's question

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Appendix A: Computationally Efficient Parameterization of the Unitary Group

If section [VIB 1](#), the SSH parameterization was introduced as a non-degenerate parameterization of the unitary group $\mathcal{U}(d)$. As presented, the SSH parameterization suffers due to the presence of computationally expensive matrix exponential terms [\[12\]](#). Although not explicitly mentioned in [\[10\]](#), it is possible to remove the reliance on matrix exponential operations in eq. [\(5\)](#) by utilizing the explicit form of the exponential terms in eq. [\(7\)](#). As a first step, recognize the defining property of the projective operators eq. [\(6\)](#),

$$P_l^k = (|l\rangle\langle l|)^k = |l\rangle\langle l| = P_l$$

This greatly simplifies the global phase terms GP_l ,

$$GP_l = \exp(iP_l\lambda_{l,l}) = \sum_{k=0}^{\infty} \frac{(iP_l\lambda_{l,l})^k}{k!} = \mathbb{1} + \sum_{k=1}^{\infty} \frac{(i\lambda_{l,l})^k}{k!} P_l^k = \mathbb{1} + P_l \left[\sum_{k=1}^{\infty} \frac{(i\lambda_{l,l})^k}{k!} \right] = \mathbb{1} + P_l (e^{i\lambda_{l,l}} - 1) \quad (\text{A1})$$

Analogously for the relative phase terms $RP_{n,m}$,

$$RP_{n,m} = \dots = \mathbb{1} + P_n (e^{i\lambda_{n,m}} - 1) \quad (\text{A2})$$

Finally, the rotation terms $R_{m,n}$ can also be simplified by examining powers of $i\sigma_{m,n}$,

$$R_{m,n} = \exp(i\sigma_{m,n}\lambda_{m,n}) = \sum_{k=0}^{\infty} \frac{(|m\rangle\langle n| - |n\rangle\langle m|)^k \lambda_{m,n}^k}{k!}$$

One can verify that the following properties hold,

$$\begin{aligned} & (|m\rangle\langle n| - |n\rangle\langle m|)^0 = \mathbb{1} \\ & \forall k \in \mathbb{N}, k \neq 0 : (|m\rangle\langle n| - |n\rangle\langle m|)^{2k} = (-1)^k (|m\rangle\langle m| + |n\rangle\langle n|) \\ & \forall k \in \mathbb{N} : (|m\rangle\langle n| - |n\rangle\langle m|)^{2k+1} = (-1)^k (|m\rangle\langle n| - |n\rangle\langle m|) \end{aligned}$$

Revealing the simplified form of $R_{m,n}$,

$$\begin{aligned} R_{m,n} &= \mathbb{1} + (|m\rangle\langle m| + |n\rangle\langle n|) \sum_{j=1}^{\infty} (-1)^j \frac{\lambda_{n,m}^{2j}}{(2j)!} + (|m\rangle\langle n| - |n\rangle\langle m|) \sum_{j=0}^{\infty} (-1)^j \frac{\lambda_{n,m}^{2j+1}}{(2j+1)!} \\ R_{m,n} &= \mathbb{1} + (|m\rangle\langle m| + |n\rangle\langle n|)(\cos \lambda_{n,m} - 1) + (|m\rangle\langle n| - |n\rangle\langle m|) \sin \lambda_{n,m} \end{aligned} \quad (\text{A3})$$

By combining the optimizations of eqs. [\(A1\)](#) to [\(A3\)](#) together we arrive at an equivalent form for eq. [\(5\)](#) that is computational more efficient.

$$U = \left[\prod_{m=1}^{d-1} \left(\prod_{n=m+1}^d R_{m,n} RP_{n,m} \right) \right] \left[\prod_{l=1}^d GP_l \right] \quad (\text{A4})$$

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