Tight and Self-Testing Multipartite Quantum Bell Inequalities from the Renormalization Group

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Attempts to understand multipartite quantum nonlocality are thwarted by the difficulty of devising quantum Bell inequalities (QBI) for systems composed of more than a few separate parties. In this Letter, we introduce the notion of *tight connectors*, a class of tensors which, if contracted according to some simple rules, result in tight QBIs. The new inequalities are saturated by tensor network states whose structure mimics the corresponding network of connectors. We further formulate the connector property of "full self-testing," which singles out a subset of tight connectors whose associated QBIs can only be saturated (modulo local isometries) by probing the corresponding tensor network state with specific measurement operators. We provide large analytic families of tight, full self-testing connectors that allow for the generation, via contraction, of N-partite QBIs with a ratio between the maximum quantum and classical values that grows exponentially with N. In turn, our method provides a modular recipe for the generation of extremal quantum behaviors and associated tight bounds in arbitrarily large systems.

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Quantum Bell inequalities and connectors—The correlations observed by distant parties measuring a joint quantum state do not, in general, admit a classical description. This is the gist of Bell's theorem [1], one of the deepest discoveries in quantum physics, which ten years ago led to several experimental disproofs of local realism [2–4]. The quantum analog of Bell's theorem is the realization by Tsirelson that quantum correlations are similarly limited [5]: on paper, one can formulate physical theories compatible with special relativity, but capable of generating stronger-than-quantum correlations [6,7]. Like their classical counterparts, limits on quantum correlations can be expressed in the form of quantum Bell inequalities (QBI), the statement that a certain linear function of the measurement statistics of a Bell experiment is bounded by some value if the experimental setup is subject to the laws of quantum mechanics. As such, QBIs limit the set of allowed statistical outputs in quantum experiments and provide falsifiability criteria for quantum theory itself, which has been tomographically tested solely on few-particle systems. In addition, an experimental Bell value close to the quantum limit can sometimes reveal important information regarding the physical system generating the correlations, such as the degree of entanglement of the underlying quantum state [8] or its local dimension [9]. In this regard, some QBIs are self-testing [10]: loosely speaking, their maximal value can only be achieved in quantum systems by measuring a specific multipartite quantum state with specific local measurement operators. Crucially, self-testing plays a key role in most security proofs of device-independent randomness generation [11,12], quantum key distribution [13,14], and delegated quantum computing [15].

There exist few general tools to construct QBIs [16–19], and the computational complexity of them all is exponential on the number of parties. To tackle the problem of generating many-body QBIs, the notion of *connectors* was introduced in Ref. [20]. In the context of quantum nonlocality, connectors are directed tensors representing coarse-graining transformations within a physical theory whose states are vectors of quantum measurement probabilities. The acyclic contraction of a number of connectors thus defines a renormalization flow within the theory, and the resulting tensor constitutes a many-body QBI. Unfortunately, while connector theory leads to sound QBIs for arbitrarily many parties, those can sometimes be very loose [20].

In this Letter, we introduce the concept of *tight connectors*, which have the property that any contraction

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thereof according to very simple rules defines a tight quantum Bell inequality. More specifically, each of the legs or indices of a tight connector is associated to a system of local measurements, and only contractions between legs with the same measurements (what we call congruent contractions) are allowed. Using existing QBIs, we construct large analytic families of tight connectors. In turn, these can then be used as building blocks for the modular construction of arbitrarily large, tight QBIs, each of which can be saturated by preparing a tensor network state [21] with the same network topology as the connectors' network. We similarly formulate the notion of *full self-testing connectors*, a subset of tight connectors whose congruent contraction defines self-testing QBIs [10]. We provide sufficient criteria to certify the full self-testing property, which apply to all tight connectors previously derived. Finally, we show that some families of full self-testing connectors generate by contraction QBIs for which the quotient between the maximal quantum and classical values increases exponentially with the system size.

The Bell scenario, connector theory, and notation—Picture a scenario where n separate labs simultaneously conduct experiments labeled by the symbols $x_1, \ldots, x_n$, obtaining the outcomes $a_1, \ldots, a_n$ with some probability $P(a_1, \ldots, a_n|x_1, \ldots, x_n)$. The vector of probabilities $P := (P(\vec{a}|\vec{x}))_{\vec{a},\vec{x}}$ is dubbed the *behavior* of the joint system. A behavior P is compatible with the laws of quantum mechanics if it can be expressed as the result of locally measuring a joint quantum system, i.e., if there exists an n-partite state ρ and positive operator valued measures (POVMs) $\{A^{(i)}_{a|x} : a\}$ such that

$$P(\vec{a}|\vec{x}) = \mathrm{Tr}\left[(A^{(1)}_{a_1|x_1} \otimes \ldots \otimes A^{(n)}_{a_n|x_n})\rho\right], \quad \forall\ \vec{a},\vec{x}. \tag{1}$$

The problem of determining if an observed behavior P is quantum (or close to) is, in general, undecidable [22]. It can be approached through quantum Bell inequalities (QBI) [5,23]: expressions of the form $\mathsf{B}(P) \leq \alpha$, where B is a linear function and the relation is supposed to hold for all quantum P.

A $q \to p$ connector C [20] is a tensor of the form $\mathsf{C}^{a_1,\ldots,a_q|x_1,\ldots,x_q}_{b_1,\ldots,b_p|y_1,\ldots,y_p}$ which, contracted with the first q legs of any n-partite quantum behavior tensor $P(\vec{a},\vec{c}|\vec{x},\vec{z})$ [here $\vec{c},\vec{z}$ are $(n-q)$-dimensional vectors of outcomes and settings], generates a (possibly non-normalized) $n+p-q$ quantum behavior

$$P'(\vec{b},\vec{c}|\vec{y},\vec{z}) = \sum_{\vec{a},\vec{x}} \mathsf{C}^{\vec{a}|\vec{x}}_{\vec{b}|\vec{y}} P(\vec{a},\vec{c}|\vec{x},\vec{z}). \tag{2}$$

Here, we only deal with $q \to 1$ connectors. Their associated coarse graining can then be also considered as an action on the measurement system $A^{(i)}$ (see Fig. 1). Specifically, we denote by $\mathsf{C}[A]$ the set of operators

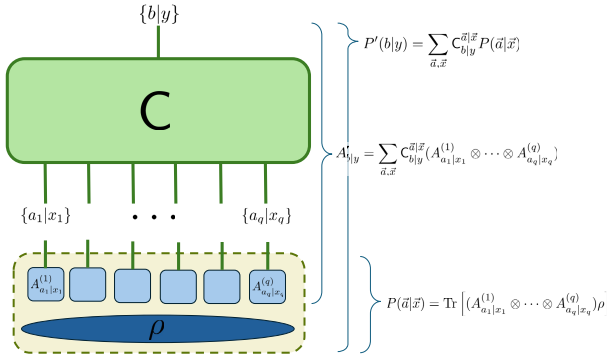


FIG. 1. Connector $\mathsf{C}^{\vec{a}|\vec{x}}_{b|y}$ can be seen as a linear transformation between probabilities $P \to P'$ [via the contraction of the corresponding indices, cf. Eq. (2)] that preserves a set of behaviors, in our case, quantum behaviors allowed by the Born rule. The action of a $q \to 1$ connector can also be interpreted as a transformation on the measurement operators $A \to A'$ [cf. Eq. (3)], inducing a renormalization flow when repeated in a larger acyclic network.

$$\mathsf{C}[A] := \left\{ \sum_{\vec{a},\vec{x}} \mathsf{C}^{a_1,\ldots,a_q|x_1,\ldots,x_q}_{b|y} A^{(1)}_{a_1|x_1} \otimes \ldots \otimes A^{(q)}_{a_q|x_q} : b, y \right\}. \tag{3}$$

Clearly, $0 \leq \mathsf{C}_{b|y}[A] \leq \mathbb{I}$ for all measurement systems A in order for C to be a valid $q \to 1$ connector. In addition, the operator $\sum_b \mathsf{C}_{b|y}[A] =: \Lambda[A]$ must be independent of y and upper bounded by $\mathbb{I}$. These two features alone suffice to define a connector [20]. If, in addition, $\Lambda[A] = \mathbb{I}$, for all sets of measurements A, we speak of a normalized connector. Any such connector will map normalized quantum behaviors to normalized quantum behaviors.

The acyclic contraction of several connectors also defines a connector. Thus, if we acyclically contract many connectors, the resulting connector C will define QBIs through $0 \leq \mathsf{C}_{b|y}[P] \leq 1$ for as many parties as uncontracted input legs. This is a simple recipe for generating multipartite QBIs [20].

In the next two paragraphs, we introduce the notion of tight connectors. To do so, it is useful to start from a simple dichotomic Bell scenario, that is, we next consider experiments with only two outputs per party, labeled $+1$ and -1. Following the tradition in the nonlocality literature, we make use of the POVM dichotomic operator $A^{(k)}_{+1|x} - A^{(k)}_{-1|x}$. From the point of view of connector theory [20], this simply corresponds to an (invertible) change of basis of the observables from the POVM elements $\{A_{a|x}\}$ to the set $\{K^{(k)}_\star := \mathbb{I}^{(k)} \equiv A^{(k)}_{+1|x} + A^{(k)}_{-1|x}\} \cup \{K^{(k)}_x := A^{(k)}_{+1|x} - A^{(k)}_{-1|x}\}$ (see End Matter for the corresponding effect of the change of basis on the connector).

A remarkable property of the CHSH functional—Consider the following two CHSH Bell functionals:

$$\mathsf{B}[K] = K_0^{(1)} \otimes K_0^{(2)} + K_1^{(1)} \otimes K_0^{(2)} + K_0^{(1)} \otimes K_1^{(2)} - K_1^{(1)} \otimes K_1^{(2)},$$
$$\mathsf{B}'[K] = -K_0^{(1)} \otimes K_0^{(2)} + K_1^{(1)} \otimes K_0^{(2)} + K_0^{(1)} \otimes K_1^{(2)} + K_1^{(1)} \otimes K_1^{(2)}. \quad (4)$$

Famously, for any classical behavior P, it holds that $|\langle \mathsf{B} \rangle_P| \leq 2$, while Tsirelson's bound [5] asserts that quantum behaviors Q satisfy $|\langle \mathsf{B} \rangle_Q| \leq 2\sqrt{2}$ (and similarly for B'). Let σ_1, σ_2, σ_3 denote the three Pauli matrices. Up to isometries, one can obtain the extreme values $\pm 2\sqrt{2}$ of B by measuring

$$\bar{K}_0^{(1)} = \sigma_3, \qquad \bar{K}_1^{(1)} = \sigma_1,$$
$$\bar{K}_0^{(2)} = \frac{\sigma_3 + \sigma_1}{\sqrt{2}}, \qquad \bar{K}_1^{(2)} = \frac{\sigma_3 - \sigma_1}{\sqrt{2}}, \quad (5)$$

on the maximally entangled states

$$|\phi_+\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}, \qquad |\psi_-\rangle = \frac{|10\rangle - |01\rangle}{\sqrt{2}}. \quad (6)$$

This means in particular that $|\phi_+\rangle$ and $|\psi_-\rangle$ are the $\pm 2\sqrt{2}$ eigenstates of the operator $\mathsf{B}[\bar{K}]$. Remarkably, $\mathsf{B}'[\bar{K}]$ also takes a particularly simple form, that is, by completing $\{|\phi_+\rangle, |\psi_-\rangle\}$ to any orthonormal basis one finds

$$\mathsf{B}[\bar{K}] = 2\sqrt{2} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$
$$\mathsf{B}'[\bar{K}] = 2\sqrt{2} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (7)$$

Hence, $\mathsf{B}[\bar{K}]$ and $\mathsf{B}'[\bar{K}]$ *effectively act* as the σ_3 and σ_1 Pauli matrices, respectively, on the subspace spanned by $\{|\phi_+\rangle, |\psi_-\rangle\}$. More precisely, defining the coisometry $V \coloneqq |0\rangle\langle\phi_+| + |1\rangle\langle\psi_-|$ we see that $V\mathsf{B}[\bar{K}]V^\dagger = 2\sqrt{2}\sigma_3$ and $V\mathsf{B}'[\bar{K}]V^\dagger = 2\sqrt{2}\sigma_1$. This gives us the idea that it is possible to feed these renormalized observables into larger Bell functionals.

Tight connectors and congruent contractions—Consider in fact the 3-party Bell functional

$$\mathsf{D}[K^{(1,2,3)}] = \mathsf{B}[K^{(1,2)}] \otimes K_0^{(3)} + \mathsf{B}'[K^{(1,2)}] \otimes K_0^{(3)} + \mathsf{B}[K^{(1,2)}] \otimes K_1^{(3)} - \mathsf{B}'[K^{(1,2)}] \otimes K_1^{(3)}. \quad (8)$$

As $|\mathsf{B}|$ is classically bounded by 2, it immediately follows that $|\mathsf{D}| \leq 4$ classically. The same argument tells us that on quantum behaviors it will hold that $|\mathsf{D}| \leq 8$. Now, the crucial point is that, due to the property (7) discussed above, we know that the quantum Bell inequality $|\mathsf{D}| \leq 8$ is again tight. To saturate it, it is sufficient to take $K^{(1,2)} = \bar{K}^{(1,2)}$, $K^{(3)} = \bar{K}^{(2)}$ and apply them on $|\tilde{\phi}_+\rangle_{123} = (|\phi_+\rangle_{12}|0\rangle_3 + |\psi_-\rangle_{12}|1\rangle_3/\sqrt{2}) \equiv V_2^\dagger |\phi_+\rangle_{23}$ to get, e.g., $\mathsf{D} = 8$.

One can interpret the above construction as the contraction of a tight connector C, which we label *Tsirelson connector*, defined (in the K basis) as $2\sqrt{2}\mathsf{C}_0[K^{(1,2)}] = \mathsf{B}[K^{(1,2)}]$, $2\sqrt{2}\mathsf{C}_1[K^{(1,2)}] = \mathsf{B}'[K^{(1,2)}]$, with itself, specifically $\mathsf{D}[K^{(1,2,3)}] = 8\mathsf{C}_0[\mathsf{C}[K^{(1,2)}], K^{(3)}]$. (we use here the correlators' basis on the measured observables; for details on the notation and how to change basis from A to K, see the End Matter). Clearly, a corresponding QBI $\mathsf{D}' = 8\mathsf{C}_1[\mathsf{C}[K^{(1,2)}], K^{(3)}]$ can be built, and the same procedure can be reiterated.

In the general case, we define a *tight connector* (cf. End Matter and Supplemental Material [24]) as a $q \to 1$ connector $\mathsf{C}[A]$ for which a set of measurements $\bar{A}$ exist such that $\mathsf{C}[\bar{A}]|_{\mathbb{S}}$ acts on some subspace $\mathbb{S}$ as a projective set of measurements $\bar{M}$ and thus saturates $0 \leq \mathsf{C}_{b|y}[A] \leq \mathbb{I}$ nontrivially whenever $\bar{M}_{b|y} \neq 0, \mathbb{I}$. Given two tight connectors $\mathsf{C}(1)$ and $\mathsf{C}(2)$, they can be *congruently contracted* when the renormalized output measurements of $\mathsf{C}(1)$ correspond to one of the optimal local input measurements of $\mathsf{C}(2)$ that is $\bar{M}(1) = \bar{A}^{(k)}(2)$ for some party k. The *congruent contraction* is thus defined as $\mathsf{C}(2)[A^{(1)}, \ldots, A^{(k-1)}, \mathsf{C}(1)[A], A^{(k+1)}, \ldots, A^{(q_2)}]$.

In particular, the example provided above shows that the Tsirelson connector can be congruently contracted with itself and generate new tight QBIs. Crucially, we prove that this is a general property (see End Matter).

Result 1—The congruent contraction of tight connectors provides a new tight connector and new associated tight QBIs.

This result immediately suggests a reiteration recipe: the congruent contraction in an acyclic network of tight connectors defines N-partite tight connectors and QBIs on the bottom N legs of the network (see Fig. 2).

Construction of tight connectors—It is now worth noticing that the construction leading to the Tsirelson connector presented above can be easily generalized: given a Bell functional B that is normalized (namely, satisfying $-\mathbb{I} \leq \mathsf{B}[K] \leq \mathbb{I}, \ \forall \ K$) and such that, for some $\bar{K}$ and some

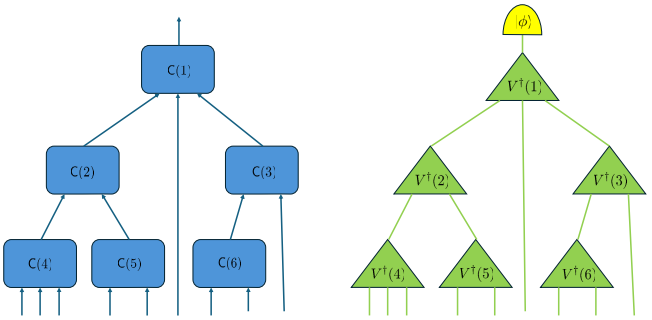


FIG. 2. Left: Bell functional obtained by congruently contracting a network of connector complexes. Each single contraction strictly reduces the number of output legs and defines a measurement renomalization. Right: tensor network state maximizing the quantum Bell functional [24]; if $|\phi\rangle$ is the $+1$ (0) eigenvector of $M(1)$, the state $V^\dagger(6)V^\dagger(5)V^\dagger(4)V^\dagger(3)V^\dagger(2)V^\dagger(1)|\phi\rangle$ saturates the quantum Bell inequality associated to the congruent contraction of the $\{\mathsf{C}(i)\}_{i=1}^6$. For the Tsirelson connector $V = |0\rangle\langle\phi_+| + |1\rangle\langle\psi_-|$.

2-dimensional subspace $\mathbb{S}$, the operator $\mathsf{B}[\bar{K}]|_{\mathbb{S}}$ has ± 1 eigenvalues, we just need to find a second normalized Bell functional B' such that $\mathsf{B}'[\bar{K}]|_{\mathbb{S}}$ also has eigenvalues ± 1. The two functionals B, B' can then be combined into a dichotomic connector.

In Supplemental Material [24], we use this construction to derive large, analytic families of 2-input–2-output connectors beyond the $2 \to 1$ Tsirelson connector presented above. More specifically, we find that we can take as a "seed QBI" B (i) any of the Tilted CHSH inequalities [25,26], which allow us to devise $2 \to 1$ connectors with subspace $\mathbb{S}$ spanned by a pair of nonmaximally entangled two-qubit states; (ii) any of the WBC Bell inequalities [27], which allow us to devise $2 \to 1$ connectors with arbitrary pairs of nonorthogonal projections associated to each of their input legs; and (iii) any of the BASTA Bell inequalities [28] for graph states, leading to $q \to 1$ connectors.

The construction above thus yields a vast set of simple tight connectors, including continuously parametrized families thereof [24].

Properties of tight connectors' congruent contractions—The multipartite QBI generated by the contraction of tight connectors enjoys several properties which we present here concisely. First, consider the congruent contraction of several tight connectors leading to a single output leg, as in Fig. 2. By constructively inverting the coisometries $V(i)$ associated to the projection on each $\mathbb{S}(i)$, [specifically, $V(i)\mathsf{C}(i)[\bar{A}(i)]V^\dagger(i) = \bar{M}(i)$; see a short explanation in the End Matter and details in Supplemental Material [24] Sec. III], it is possible to prove the following.

Result 2—The state saturating the extremal value of a tight quantum Bell inequality obtained via the contraction of tight connectors with a single output leg is a tensor network state obtained from the same network topology.

Second, consider once again the Tsirelson connector described in the previous section. The CHSH functional has maximum value $2\sqrt{2}$, while the corresponding classical bound is 2. As we discussed, by contracting the Tsirelson tensor with itself, the corresponding inequality (8), thanks to tightness, has a saturable quantum bound equal to $(2\sqrt{2})^2 = 8$, while being classically bounded by $2^2 = 4$. By reiterating the contraction, one obtains that the ratio between the quantum and classical maximal value of the corresponding N-partite Bell inequality grows exponentially as $\sqrt{2}^{(N-1)}$. In Supplemental Material [24] (Sec. V) we prove that this is a general property of connectors based on *XOR-game Bell inequalities* [29], namely, Bell inequalities that can be written as a linear combination of q-partite correlator products, $\mathsf{B}[K] = \sum_{x_1,\ldots,x_q} c_{x_1,\ldots,x_q} \otimes_{k=1}^q K_{x_k}^{(k)}$ (several of the connectors generated via the two-dimensional construction presented above are of this form).

Result 3—The contraction of tight connectors built via multipartite XOR games generates QBI with a quantum to classical ratio that grows exponentially in the total number of parties N.

In Supplemental Material [24] we characterize the geometrical factors associated to each XOR-type connector, which in turns provides a rule for designing contractions with the highest possible quantum to classical gap.

Finally, we comment on how the Bell inequalities constructed via the congruent contraction of connector complexes can be used to *self-test* the underlying quantum state and measurements. Self-testing refers to the remarkable feature of certain Bell inequalities, whose maximum violation uniquely fixes the experimental state and local operators, modulo local isometries; see Ref. [10] for a review. A few results have been obtained in the literature, e.g., notably the fact that all pure bipartite entangled states can be self-tested [30], as well as all real projective measurements [31]. More recently, the authors of Ref. [32] proved that all pure multipartite qubit states can be self-tested up to complex conjugation.

In Supplemental Material [24] we introduce a notion of self-testing that is slightly stronger than the one typically found in the literature: essentially, we denote a QBI to be *full self-testing* when its maximum value certifies (modulo local isometries) not just the underlying quantum state and the action of the measurement operators over it but also the action of the measurement operators over the full, underlying Hilbert space (see End Matter for a formal definition). Despite the fact that full self-testing is the strongest form of self-testing ever proposed in the literature [10], we provide a simple, sufficient criterion to promote a standard self-testing result to a full self-testing result [24].

We also propose a definition of *self-testing connectors*: in a nutshell, a self-testing $q \to 1$ connector C is a tight connector for which $\sum_{b,y} \mu_{b,y} \mathsf{C}_{b|y}[\mathsf{A}]$ is a full self-testing QBI, for some vector μ; see the End Matter for the complete

definition. Crucially, we are able to prove, in Supplemental Material [24] (Sec. VI), the following.

Result 4—The congruent contraction of full self-testing connectors is a full self-testing connector.

Hence, one can generate full self-testing, multi-partite QBI through the contraction of a network of full self-testing connectors.

All of the above invariably leads to two questions: Are there full self-testing QBI? Are there full self-testing connectors? In this regard, applying our sufficiency criteria for full self-testing to the objects constructed above, we find the following.

Result 5—All tight connector families introduced in Supplemental Material [24] are full self-testing, with $\mu_{b,y} = \delta_{b,b_0}\delta_{y,y_0}$, for any b_0, y_0.

In particular, all of the tight QBIs constructed by contracting the tight connectors identified so far self-test the associated tensor network states, as well as the local measurements in the uncontracted input legs.

A modular recipe for extremal quantum behaviors—In this Letter, we introduced the notion of tightness in connector theory. In a nutshell, a $q \to 1$ normalized connector is tight if all of its associated q-partite QBI can be saturated with the same measurement operators. This requirement makes the congruent contraction of any number of tight connectors result in another tight connector, from which one can derive new, multipartite tight QBI. Moreover, such inequalities, which are maximally violated by tensor network states [21], can be shown to be self-testing if each of the tight connectors involved satisfies an extra, verifiable property, which we dubbed full self-testing.

To our surprise, instances of tight, full self-testing connectors can be constructed from the oldest quantum Bell inequality: Tsirelson's bound [5]. Notably, we also show [24] that recently discovered self-testing QBIs [25,27,33] can be similarly used to build families of tight, full self-testing connectors. Moreover, one such family generates, by contraction, XOR Bell functionals for which the ratio between the maximum quantum and classical values increases exponentially with the system size.

All in all, our results provide a flexible modular recipe for the construction of arbitrarily large QBIs and corresponding extremal quantum correlations that enjoy several remarkable properties, starting from simple building blocks. An example based entirely on the self-contraction of the Tsirelson connector is provided in Fig. 3, while others can be found in Supplemental Material [24]. For future research, now that we have large families of tight connectors, the next logical step is exploring their potential to generate *local* QBIs, in the manner sketched in Ref. [34].

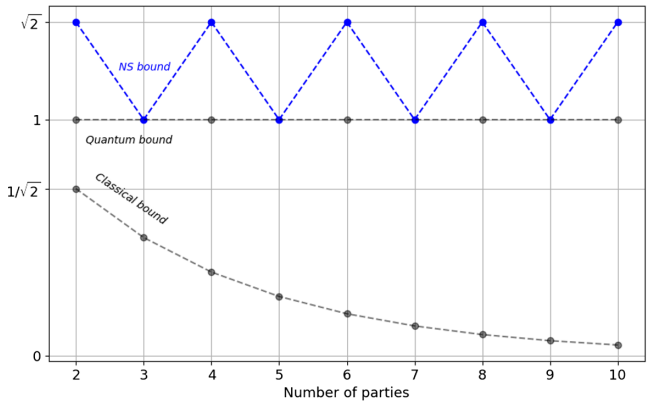


FIG. 3. Maximum values for the Bell functional resulting from the recursive self-contraction of the Tsirelson connector with itself, which is normalized by construction to 1 for quantum behaviors. The exponential decay in the size of the classical bound is a property of any network based on XOR-type connectors (cf. Result 3), whereas the maximum value attained by general no-signalling behaviors remains bounded by $\sqrt{2}$. In the case of a network constructed using Tsirelson connectors only, the classical (as well as the quantum) bound is independent on the specific contraction geometry used, and the same appears to be true (empirically) for the no-signaling bound.

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Data availability—There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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End Matter

Tight connectors and congruent contractions—Consider a $q \to 1$ quantum connector C, acting as indicated in Eq. (2), with the property that, for some Hilbert spaces $H_1, \ldots, H_q$ and some measurement operators $\{\bar{A}^{(k)}_{a|x} : a, x\} \subset B(H_k)$, there exists a coisometry $V : \bigotimes_k H_k \to H$ such that the operators $\bar{M}_{b|y} \in B(H)$, defined by

$$\bar{M}_{b|y} := V \mathsf{C}_{b|y}[\bar{A}] V^\dagger, \tag{A1}$$

are projectors satisfying $\sum_b \bar{M}_{b|y} = \mathbb{I}_H$, for all y. Then we say that C is a *tight connector*. The name stems from the fact that, for all $\bar{M}_{b|y} \neq 0, \mathbb{I}$, the QBIs

$$0 \leq \mathsf{C}_{b|y}[A] \leq 1 \tag{A2}$$

are tight. In particular, the value 1 (0) can be achieved with the operators $\bar{A}$ and any state of the form $V^\dagger|\phi\rangle$, with $\bar{M}_{b|y}|\phi\rangle = |\phi\rangle$ ($\bar{M}_{b|y}|\phi\rangle = 0$).

Definition—(Connector complex). We define a *connector complex* as a tuple $\mathcal{C} \coloneqq (\mathsf{C}, \bar{A}, V)$ [where $\mathsf{C}(\mathcal{C})$ is a connector, $\bar{A}$ is a system of measurement operators, and V is a coisometry], such that Eq. (A1) is satisfied for some projective measurement system $\bar{M}$ (implying that C is tight). In the following, we use $\mathsf{C}(\mathcal{C})$, $\bar{A}(\mathcal{C})$, and $V(\mathcal{C})$ to denote the elements of the tuple $\mathcal{C}$. The symbols $\bar{M}_{b|y}(\mathcal{C})$, $H_k(\mathcal{C})$, and $H(\mathcal{C})$ will similarly have obvious meanings.

Notice that, if $\mathcal{C} = (\mathsf{C}, \bar{A}, V)$ is a connector complex, then so is $\mathcal{C}' = [\mathsf{C}, (U^{(k)}\bar{A}^{(k)}U^{(k)\dagger})_k, WV \otimes_k U^{(k)\dagger}]$ for any unitaries $U^{(1)}, \ldots, U^{(q)}, W$. Complexes $\mathcal{C}$ and $\mathcal{C}'$ will be said to be unitarily equivalent.

Call $I(\mathcal{C})$ the space spanned by vectors of the form $V(\mathcal{C})^\dagger|\beta\rangle \in \otimes_k H_k$ (where $|\beta\rangle \in H$). Note that, since $\mathsf{C}_{b|y}[\bar{A}]$ is an effect and its submatrix $\bar{M}_{b|y}$ is a projector, it follows that $\mathsf{C}_{b|y}(\bar{A})I(\mathcal{C}) \subset I(\mathcal{C})$. Thus we call $I(\mathcal{C})$ the *invariant subspace* of $\mathcal{C}$.

Consider two connector complexes $\mathcal{C}_1, \mathcal{C}_2$, and suppose that we contract the output leg of $\mathsf{C}(\mathcal{C}_1)$ with the k^{th} input legs of $\mathsf{C}(\mathcal{C}_2)$, as in Fig. 4. We call this contraction *congruent* if $\bar{M}(\mathcal{C}_1) = \bar{A}^{(k)}(\mathcal{C}_2)$ [this means in particular that $\bar{A}^{(k)}(\mathcal{C}_2)$ is a system of projective measurements]. Any congruent contraction of the connectors of two connector complexes results in a tight connector.

Let us see why this occurs (refer to Fig. 4 for a visual representation): call C the result of contracting the tensors

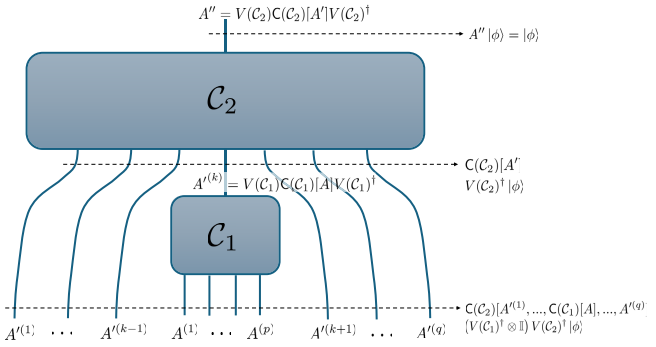


FIG. 4. Result of using the output of a $p \to 1$ connector $\mathsf{C}(\mathcal{C}_1)$ as the kth input of a $q \to 1$ connector $\mathsf{C}(\mathcal{C}_2)$ is a $p + q - 1 \to 1$ connector. A connector is tight if for some choice of measurements $\bar{A}$ and some coisometry V, the "renormalized" measurement $A' = V\mathsf{C}[\bar{A}]V^\dagger = \bar{M}$ is projective. This ensures that the Bell inequality $0 \le \mathsf{C}[A] \le 1$ is tight and can be saturated by applying $V^\dagger$ to the corresponding eigenvector of M (see text). The set $\mathcal{C} = \{\mathsf{C}, \bar{A}, V\}$ then defines a *connector complex*. When the renormalized measurement coincides with the optimal input measurement $\bar{A}'$ of the following connector $\mathsf{C}(\mathcal{C}_2)$, the complexes $\mathcal{C}_1$ and $\mathcal{C}_2$ can be *congruently contracted*, resulting in another tight connector complex. This allows for backpropagating the saturation of any of the (trivial) QBI associated to the final output leg—say $A'' \le 1$—and its optimal eigenvector $|\phi\rangle$, to the corresponding QBI on A' and A and their saturation strategies, via the sequential application of the isometries $V_2^\dagger$ and $V_1^\dagger$.

$\mathsf{C}(\mathcal{C}_1), \mathsf{C}(\mathcal{C}_2)$ of the two complexes. Then we have that C is a connector as it is the contraction of two connectors [20]. Next, define the coisometry

$$V = V(\mathcal{C}_2)\left(\bigotimes_{j<k}\mathbb{I}^{(j)} \otimes V(\mathcal{C}_1) \otimes \bigotimes_{j>k}\mathbb{I}^{(j)}\right), \tag{A3}$$

where $\mathbb{I}^{(j)}$ denotes the identity operator in the Hilbert space $[H_j(\mathcal{C}_2)]$. It is easy to see that V satisfies Eq. (A1), with $\bar{M}_{b|y} = \bar{M}_{b|y}(\mathcal{C}_2)$ and

$$\begin{aligned} &\bar{A}^{(j)}_{a|x} = \bar{A}^{(j)}_{a|x}(\mathcal{C}_2), \quad \text{for } j < k, \\ &\bar{A}^{(j-k+1)}_{a|x}(\mathcal{C}_1), \quad \text{for } k \le j < k + q(\mathcal{C}_1), \\ &\bar{A}^{(j-q(\mathcal{C}_1)+1)}_{a|x}(\mathcal{C}_2), \quad \text{for } j \ge k + q(\mathcal{C}_1). \end{aligned} \tag{A4}$$

Since $M(\mathcal{C}_2)$ represent projective measurements, we have that the tuple $\mathcal{C} = (\mathsf{C}, \bar{A}, V)$ is a connector complex. We dub $\mathcal{C}$ the (congruent) contraction of complexes $\mathcal{C}_1, \mathcal{C}_2$.

Now, think of a network of connector complexes, congruently contracted in a treelike graph with just one root. By the previous argument, this defines a connector complex $\mathcal{C}$, so $\mathsf{C} = \mathsf{C}(\mathcal{C})$ is tight. Hence, for any quantum Bell inequality of the form (A2), the upper [lower] bound is guaranteed to be tight if $\bar{M}_{b|y}(\mathcal{C}) \neq 0$ [$\bar{M}_{b|y}(\mathcal{C}) \neq \mathbb{I}$]. Both upper and lower bounds can be achieved with measurements $\bar{A}(\mathcal{C})$ and states of the form $V^\dagger(\mathcal{C})|\phi\rangle$, with $|\phi\rangle$ being an eigenvector of $\bar{M}_{b|y}(\mathcal{C})$ with eigenvalue 1 or 0, depending on the bound that we wish to saturate.

Remarkably, from the composition of coisometries (A3), it follows that the optimal state $|\psi\rangle$ is a tensor network state: to generate it, one just needs to apply to $|\phi\rangle$ a sequence of local isometries, whose contraction structure mimics that of the connectors; see Fig. 2 and Supplemental Material [24].

Measurement to correlator basis in dichotomic scenarios—Consider connectors and Bell functionals with indices $a|x$ such that a can just take the values -1, 1. In this case, it can be more convenient to express the outgoing index of each connector in a basis that, rather than referring to the measurement operators $\{A_{a|x}\}$, points to the corresponding dichotomic operators $\{K_\star = \mathbb{I}\} \cup \{K_x\}$, where $K_x \coloneqq A_{+1|x} - A_{-1|x}$. This choice of basis formally consists in relabeling the values of the outgoing index or leg of a connector from $a|x$, to $\star, x$, with $\star$ (x) representing $\mathbb{I}$ (K_x). The change of basis for a connector C is as follows:

$$\mathsf{C}_\star \coloneqq \sum_{b=-1,1} \mathsf{C}_{b|y}, \qquad \mathsf{C}_y \coloneqq \sum_{b=-1,1} \mathsf{C}_{b|y} b. \tag{B1}$$

The inverse transformation is given by

$$\mathsf{C}_{b|y} = \frac{1}{2}(\mathsf{C}_\star + b\mathsf{C}_y). \tag{B2}$$

The notion of full self-testing—We next formulate a variant of self-testing that is slightly stronger than the one commonly found in the literature. To do so, we use the concept of *tensor polynomial* [35,36]. A tensor polynomial of variables $\{A^{(k)}_{a|x}\colon a, x\}_{k=1}^{q}$ is a sum of products of expressions of the form $\mathbb{I}^{(1)} \otimes \ldots \otimes \mathbb{I}^{(k-1)} \otimes A^{(k)}_{a|y} \otimes \mathbb{I}^{(k+1)} \ldots \otimes \mathbb{I}^{(q)}$. The degree of the tensor polynomial will be given by the maximum number of products within all factors k, e.g., the degree of the tensor polynomial $A^{(1)}_{0|1} \otimes A^{(2)}_{1|2}A^{(2)}_{2|3} + 5\mathbb{I}^{(1)} \otimes A^{(2)}_{1|2}$ is 2.

Armed with this notion, the definition of full self-testing is as follows:

Definition—(Full self-testing). Let $\bar{A}$ be a q-partite collection of projective measurements, with Hilbert spaces $H_1, \ldots, H_q$, and let $|\bar{\psi}\rangle \in \otimes_k H_k$ be a normalized vector such that

$$\{f[\bar{A}]|\bar{\psi}\rangle\colon f, \text{ tensor polynomial}\} = \bigotimes_k H_k. \tag{C1}$$

Given a q-partite normalized Bell functional B, we say that it *fully self-tests* $(|\bar{\psi}\rangle, \bar{A})$ if $\mathsf{B}[P] = 1$, which implies that, for any quantum realization (ψ, A), with $A^{(k)}_{a|x}\colon H'_k \to H'_k$, there exist an orthonormal basis $\{|i_k\rangle\colon i_k\}$ for each H_k, and orthonormal states $\{|\psi(i_1, \ldots, i_q)\rangle\colon i_k = 1, \ldots, \dim(H_k)\} \subset H' := \otimes_k H'_k$ satisfying

$$|\psi\rangle = \sum_{\vec{i}} \langle i_1, \ldots, i_q|\bar{\psi}\rangle|\psi(i_1, \ldots, i_q)\rangle \tag{C2}$$

and local isometries $U_1, \ldots, U_q$ such that

$$\begin{aligned} &U_1 \otimes \ldots \otimes U_q \bigotimes_k A^{(k)}_{a_k|x_k}|\psi(i_1, \ldots, i_q)\rangle \\ &\quad = \bigotimes_k \bar{A}^{(k)}_{a_k|x_k}|i_1, \ldots, i_q\rangle|\text{junk}\rangle \end{aligned} \tag{C3}$$

holds for all $a_1, x_1, \ldots, a_q, x_q, i_1, \ldots, i_q$.

Contrary to standard self-testing [10], in full self-testing the "actual" measurement system A is not assumed to be projective; on the contrary, for any k, x, we allow $(A^{(k)}_{a|x})_a$ to be a general POVM.

Remarks—Equations (C2) and (C3) imply that, for any tensor polynomial $f[A]$, it holds that

$$U_1 \otimes \ldots \otimes U_q f[A]|\psi(i_1, \ldots, i_q)\rangle = f[\bar{A}]|i_1, \ldots, i_q\rangle|\text{junk}\rangle. \tag{C4}$$

Indeed, by Eq. (C3), for all tensor polynomials g of degree 1, we have that $Ug[A]|\psi(i_1, \ldots, i_q)\rangle = \sum_{\vec{j}} \langle \vec{j}|g[\bar{A}]|\vec{i}\rangle|\vec{j}\rangle|\text{junk}\rangle$, with $U = U_1 \otimes \ldots \otimes U_q$. Multiplying on both sides by $U^\dagger$, one obtains $g[A]|\psi(i_1, \ldots, i_q)\rangle = \sum_{\vec{j}} \langle \vec{j}|g[\bar{A}]|\vec{i}\rangle|\psi(\vec{j})\rangle$. By induction, we have that $\prod_k g_k[A]|\psi(i_1, \ldots, i_q)\rangle = \sum_{\vec{j}} \langle \vec{j}|\prod_k g_k[\bar{A}]|\vec{i}\rangle|\psi(\vec{j})\rangle$, for any tuple of tensor polynomials $(g_k)_k$ of local degree 1. The general relation (C4) follows by linearity.

Moreover, it clearly follows from Eqs. (C2) and (C3) that

$$U_1 \otimes \ldots \otimes U_q \bigotimes_k A^{(k)}_{a_k|x_k}|\psi\rangle = \bigotimes_k \bar{A}^{(k)}_{a_k|x_k}|\bar{\psi}\rangle|\text{junk}\rangle. \tag{C5}$$

These remarks make full self-testing—to our knowledge-the–strongest notion of (device-independent) quantum certification in the literature as it certifies the underlying state and the action of the measurements *component-wise* in some basis. In particular full self-testing clearly implies standard self-testing (C5) [10] for general (nonprojective) operator systems A.

The definition of full self-testing is extended to connectors in the following way:

Definition—(Connector's full self-testing). The $q \to 1$ connector complex $\mathcal{C}$ is *full self-testing* if there exist coefficients $\{\mu_{b|y}\colon b, y\}$ such that the Bell functional

$$\sum_{b,y} \mu_{b|y} \mathsf{C}^{b|y}(\mathcal{C})[A] \tag{C6}$$

is a normalized quantum Bell inequality that fully self-tests $[|\bar{\psi}\rangle, \bar{A}(\mathcal{C})]$, for some state $|\bar{\psi}\rangle \in I(\mathcal{C})$ and, moreover,

$$I(\mathcal{C}) = \{f[\mathsf{C}[\bar{A}]]|\bar{\psi}\rangle\colon f, \text{ tensor polynomial}\}, \tag{C7}$$

with $\mathsf{C} = \mathsf{C}(\mathcal{C})$. This condition is equivalent to $f[M(\mathcal{C})]V(\mathcal{C})|\bar{\psi}\rangle$ generating the whole range of $V(\mathcal{C})$. In the following, we denote $\mu, \bar{\psi}$ by $\mu(\mathcal{C}), \bar{\psi}(\mathcal{C})$.

Of course, if a connector complex $\mathcal{C}$ is fully self-testing, any other unitarily equivalent complex will also be.

In Supplemental Material [24] we provide verifiable conditions to prove that a Bell inequality (or connector) is full self-testing, and we crucially demonstrate that the congruent contraction of full self-testing connector complexes is itself full self-testing.