

All-multipartite Bell-correlation inequalities for two dichotomic observables per site

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We construct a set of 2^{2^n} independent Bell-correlation inequalities for n -partite systems with two dichotomic observables each, which is complete in the sense that the inequalities are satisfied if and only if the correlations considered allow a local classical model. All these inequalities can be summarized in a single, albeit nonlinear inequality. We show that quantum correlations satisfy this condition provided the state has positive partial transpose with respect to any grouping of the n systems into two subsystems. We also provide an efficient algorithm for finding the maximal quantum-mechanical violation of each inequality, and show that the maximum is always attained for the generalized GHZ state.

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I. INTRODUCTION

Entanglement has not only been a key issue in the ongoing debate about the foundations of quantum mechanics, started by Einstein, Podolsky, and Rosen in 1935 [1], it also plays a crucial role in the young field of quantum information theory. Here entangled states are one of the basic ingredients of quantum information processing, due to their role as a resource in quantum key distribution, super dense coding, quantum teleportation, and quantum error correction (cf. [2]). Although general structural knowledge about entanglement has improved dramatically in the last few years, there are still many open problems. For example, there is still no efficient general method to decide whether a given state is entangled or not.

The first, and for a long time also the only, mathematically sharp criteria for entanglement were the Bell inequalities [3]. They provided the first possibility to distinguish experimentally between quantum-mechanical predictions and those of local realistic models. But although Bell inequalities have been known for more than 30 years [4], our knowledge about the precise border between the classical and quantum-mechanical accessible region is still mainly restricted to the simplest nontrivial cases. Best known is the case of two sites, at each of which two dichotomic observables are chosen. This is characterized *completely* by the Clauser-Horne-Shimony-Holt (CHSH) version of Bell's inequalities [5], in the sense that the inequalities are satisfied if and only if a local classical model exists [6]. Finding a complete set of linear inequalities in more complicated situations (more sites, more observables, more outcomes) turns out to be a very difficult problem in the sense of computational complexity [7]. There is only very little knowledge about Bell-type inequalities beyond the CHSH case [8–12]. Though numerical studies yield a large number of inequalities [13], for most of them it is neither known by how much they can be violated in quantum theory nor is there a general characterization admitting further investigations.

We were therefore quite surprised ourselves at finding an

infinite sequence of multipartite correlation settings for which we could develop the theory to be as explicit and complete as in the CHSH case. Our setting generalizes the CHSH setting to an arbitrary number n rather than two different sites, but retains the constraints of just two observables per site with just two outcomes each. Thus each of the n participants has the choice of two observables, each of which can take the values $+1$ or -1 . For any choice of observables we then consider the expectation value of the product of all n signs (a “full” correlation function). A Bell inequality is a linear constraint on the set of all such expectations, which is valid whenever the correlations can be obtained from a local classical model, and which cannot be written as a convex combination of other such constraints. Examples are the CHSH inequality [5] for $n=2$ and their generalizations going back to Mermin and others [8–11] leading to a single inequality for arbitrary n .

We remark that this problem setting could be generalized to include the expectations not only of the product of all n signs, but also the products of subsets of signs (“restricted” correlation functions). These data would be sufficient to reconstruct the full joint probability distributions of signs for all choices of observables. However, most of the derivations in this paper do not generalize to this setting, and it is not yet clear which statements would still be valid (maybe with a different proof). When we talk of the existence of a classical model, however, it is understood that such a model would also determine all restricted correlation functions. The omission of restricted correlation functions from our setting only means that we do not consider constraints depending on them.

For this class of multipartite correlations we obtained the following results.

(i) We construct a set of 2^{2^n} Bell inequalities, and show its completeness: the correlations considered allow a local classical model if and only if all these inequalities are satisfied (Sec. III).

(ii) The convex set of collections of classical correlation functions is a 2^n -dimensional hyperoctahedron, which can be described alternatively by a single nonlinear inequality (Sec. III).

(iii) We discuss the symmetries connecting different in-

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equalities and develop a construction scheme, which yields all 2^{2^n} equalities by successive substitutions into the CHSH inequality (Sec. IV).

(iv) We reduce the computation of the maximal quantum violations of each Bell inequality to a simple variational problem with just one free variable per site. The maxima are already attained in qubit systems, more specifically for the n -party generalization of the GHZ state [15], with a choice of observables depending on the inequality under consideration (Sec. V).

(v) We extend this method to a characterization of the convex body of quantum-mechanically attainable correlation functions in terms of its extreme points, which are also found in the generalized GHZ state. These results are analogous to those of Tsirelson [16,17] for the bipartite case.

(vi) We characterize the Mermin inequality as that Bell inequality, which can be violated by the widest margin in quantum theory.

(vii) Section VI settles the relationship between the correlation Bell inequalities and another important entanglement property. We show that for states having positive partial transposes with respect to all their subsystems, all 2^{2^n} inequalities are satisfied, so the correlations in such quantum states can be explained in the context of a local realistic model. This extends our earlier result [18] for Mermin's inequalities, and is further supporting evidence for a recent conjecture by Peres [19], namely that positivity of partial transposes should generally imply the existence of local realistic models.

In the Appendix we will discuss some of the general results obtained in Secs. III, IV, and V in more detail for the special cases $n=3,4$.

II. BELL'S INEQUALITIES AND CONVEX GEOMETRY

Before entering the discussion of Bell inequalities in our special context it is useful to recall some geometric structures of the general problem and basic facts concerning the duality of convex polytopes. Consider a system decomposed into n independent subsystems. Suppose further that on each of these subsystems one out of m v -valued observables is measured. Thus each of the m^n different experimental setups may lead to v^n different outcomes, so that the raw experimental data are made up of $(mv)^n$ probabilities. These numbers form a vector ξ lying in a space of dimension $(mv)^n$ (minus a few for normalization constraints). Classically, in a local realistic model, ξ would be generated by specifying probabilities for each classical *configuration*, i.e., for every assignment of one of the v values to each of the nm observables. Here the "local" character of the theory is expressed by the property that the assignment of a value to an observable at site k does not depend on the observables chosen at other sites. Every configuration c also represents a possible classical (ideally prepared) state, and hence a vector ϵ_c of probabilities. The classical accessible region, which we will denote by Ω , is thus the convex hull of $v^{(nm)}$ explicitly known extreme points. Even though the number of configurations is large, it is finite, hence Ω is a *polytope*.

Like every compact convex set, Ω is the intersection of

all half spaces containing it. A half space is completely characterized by a linear inequality, so we must look for vectors β such that $\langle \beta, \xi \rangle \leq 1$ for all $\xi \in \Omega$. Since this property can be checked on the extreme points ϵ_c we must look at the convex set

$$\mathcal{B} = \{ \beta | \forall c: \langle \beta, \epsilon_c \rangle \leq 1 \}, \quad (1)$$

also known as the *polar* of $\{ \epsilon_c \}$. For each $\beta \in \mathcal{B}$ the inequality $\langle \beta, \xi \rangle \leq 1$ is thus a necessary condition for $\xi \in \Omega$. Moreover, the bipolar theorem [20] says that the collection of all these inequalities is also sufficient.

Luckily, the inequalities are not all independent, since the inequality for a convex combination $\beta = \sum \lambda_i \beta_i$, with $\beta_i \in \mathcal{B}$ already follows from the inequalities for the β_i . It therefore suffices to take only the extreme points of \mathcal{B} . For a polytope this has a very intuitive geometrical interpretation: the half spaces determined by extreme points touch Ω in a face of maximal dimension. Moreover, there are only finitely many such maximal faces, which is to say that \mathcal{B} is also a polytope.

The task of finding all Bell inequalities is therefore a special instance of a standard problem in convex geometry, known as the *hull problem*: given the extreme points $\{ \epsilon_c \}$ of a polytope Ω , find its maximal faces or, equivalently, the extreme points of its polar.

The duality between \mathcal{B} and Ω is a generalization of the duality between regular platonic solids, under which dodecahedron and the icosahedron, as well as the octahedron and the cube are polars of each other. A generalized (d -dimensional) octahedron is the unit sphere in a sequence space $l^1(\{1, \dots, d\})$. Its polar is the unit sphere in the dual Banach space $l^\infty(\{1, \dots, d\})$, i.e., a d -dimensional hypercube. This is precisely the situation we will find for the classically accessible region considered in this paper, where $d = 2^n$.

The first to consider the construction of a complete set of Bell-type inequalities as a problem in convex geometry apparently was M. Froissart [21]. Unfortunately, however, a general solution for all (n, m, v) is highly unlikely to exist. To find some extreme points of Eq. (1) is not so difficult, but algorithms providing the complete set are likely to run into serious growth problems already for very small (n, m, v) . In fact, there is a theorem by Pitowsky [7] to the effect that, in a closely related problem, finding all inequalities would also solve some known hard problems in computational complexity (this is in fact strongly connected with the notorious $NP=P$, respectively $NP=coNP$ questions). Pitowsky and Svozil [13] have recently performed an extensive numerical search for $n=3$, and published their result, the coefficients of 53 856 inequalities on their website. Unfortunately, there is not much generalizable insight coming out of this kind of work, but it is nice to see what can be done in this hard numerical problem. Moreover, a numerical approach based on linear optimization methods for investigating the case $(n, m, v) = (2, 2, v)$ without explicitly constructing extremal inequalities was proposed in [14]. For further problems and partial results in this genre we refer to the problem page [12] on our own website. In what follows we will restrict to the

case $(n,m,v)=(n,2,2)$ and “full” correlation functions in the sense described in the Introduction.

III. ALL BELL-CORRELATION INEQUALITIES

A. Basic notation

Talking about Bell inequalities one usually has in mind inequalities of the CHSH form [5]. These inequalities refer to correlation experiments, in which each of two parties has the choice of two ± 1 valued observables to be measured, i.e., $(n,m,v)=(2,2,2)$. Focusing only on full correlation functions for multiparticle generalizations of such systems [$(n,m,v)=(n,2,2)$, n fixed arbitrarily] the raw experimental data are 2^n expectation values, each corresponding to a different experimental setup. Each setup is labeled by the choice of observables at each site. We parameterize these choices by binary variables $s_k \in \{0,1\}$ so that s_k indicates the choice of the ± 1 -valued observable $A_k(s_k)$ at site k . Each full correlation function is thus the expectation of a product $\prod_k A_k(s_k)$, and is labeled by a bit string $s=(s_1, \dots, s_n)$.

We will consider these expectations as the components $\xi(s)$ of a vector ξ in a 2^n -dimensional space. Then any Bell inequality is of the form

$$\sum_s \beta(s) \xi(s) \leq 1, \quad (2)$$

where we have normalized the coefficients β so that the maximal classical value is 1, in accordance with the definition of polars in Sec. II. The linear combination in Eq. (2) can also be computed under the expectation value, so that this inequality can be stated as an upper bound on the expectation of

$$B = \sum_s \beta(s) \prod_{k=1}^n A_k(s_k). \quad (3)$$

We call such expressions *Bell polynomials*. They can be used directly in the quantum case, where all variables $A_k(s_k)$ are substituted by operators with $-1 \leq A_k(s_k) \leq 1$, acting in the Hilbert space of the k th site, and the product is taken as the tensor product. It is often useful to consider these polynomials rather than the set of coefficients, because often many coefficients are zero, and we can sometimes simplify a polynomial algebraically (e.g., by factorization), even though this may not be apparent from the coefficients.

Two convex sets in the real 2^n -dimensional vector space are the subject of our investigation: firstly, the polytope Ω of correlation vectors ξ coming from local classical models, and secondly the set $\mathcal{Q} \supset \Omega$ of such vectors arising from quantum models. Ω will be characterized in terms of Bell inequalities in this section, \mathcal{Q} will be considered in Sec. V.

B. Construction and completeness

In a local classical model every observable $A_k(s_k)$ is a random variable in its own right, i.e., it is a function of the “hidden variable” which does not depend on the choices s_l of observables at other sites $l \neq k$. A model must assign probabilities to any collection of values for these observables,

i.e., to each *classical configuration*. Since the extremal choices of such probabilities just assign probability 1 to one configuration and zero probability to all others, the extreme points of Ω are simply labeled by the configurations.

One configuration c is the choice of $c_k(s_k) \in \{-1,1\}$ for all k and s_k . Clearly, there are 2^{2^n} such configurations. The corresponding correlation vector $\xi \equiv \epsilon_c$ has components

$$\epsilon_c(s) = \prod_{k=1}^n c_k(s_k). \quad (4)$$

Since we only consider full correlation functions (and not restricted ones, see the Introduction), different classical configurations may give the same extreme point ϵ_c . For example, we may choose two different sites, and change the values of all $c_k(s_k)$ at these sites simultaneously. Then in Eq. (4) the sign changes cancel for all s . This is also apparent from the factorization

$$\epsilon_c(s) = \left(\prod_{k=1}^n c_k(0) \right) \prod_{l=1}^n c_l(0) c_l(s_l), \quad (5)$$

in which the first factor is just an s -independent sign, and in the second factor it suffices to choose configurations with $c_k(0)=1$. Thus we can write $c_k(s_k) = (-1)^{s_k r_k}$ with $r_k \in \{0,1\}$. Then

$$\epsilon_c(s) = \pm (-1)^{\langle r, s \rangle}, \quad \langle r, s \rangle = \sum_{k=1}^n r_k s_k, \quad (6)$$

where the extreme points are now labeled uniquely by the bit string $r=(r_1, \dots, r_n)$ and the overall sign. This leaves us with exactly 2^{n+1} extreme points of Ω .

Our task is now to find the extremal linear inequalities β , characterizing this set, i.e., the extreme points of \mathcal{B} from Eq. (1). The bipartite case was indeed completely analyzed by Fine [6], who showed that there are only two classes of inequalities: one is trivial in the sense that it just requires correlations to be in $[-1, +1]$, and the second consists of the CHSH-type inequalities, for which the prototype is $\beta = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$. A construction of some Bell-type inequalities for arbitrary n was first proposed by Mermin [8] and further developed by Ardehali [9], Belinskii and Klyshko [10], and Gisin and Bechmann-Pasquinucci [11].

We will now find *all* extremal solutions β to the set of inequalities

$$-1 \leq \sum_s \beta(s) (-1)^{\langle r, s \rangle} \leq 1, \quad (7)$$

where $r \in \{0,1\}^n$ runs over all bit strings characterizing the configurations. Suppose that of these 2^n inequalities $p < 2^n$ fixed ones are “tight” in the sense that the sum takes one of the extreme values ± 1 . This will be consistent with a plane (affine manifold) of vectors β of dimension at least $2^n - p$. We can now construct convex decompositions of β in an open neighborhood of β in this plane, since each one of the remaining sums is continuous in β , and there is a finite margin before another inequality becomes violated. This contradicts extremality, so we conclude that the inequality must be tight for all r . Thus we have 2^n signs $f(r) \in \{+1, -1\}$ with

$$\sum_s \beta(s) (-1)^{\langle r,s \rangle} = f(r). \quad (8)$$

Now we can read Eq. (8) as a Fourier transform with respect to the group of n -tuples of $\{0,1\}$ with addition modulo 2. Therefore, we easily obtain the entire set of extremal β by applying the inverse transformation to the set of vectors $f \in \{-1,1\}^{2^n}$:

$$\beta(s) = 2^{-n} \sum_r f(r) (-1)^{\langle r,s \rangle}. \quad (9)$$

These are the coefficients of the complete set of 2^{2^n} extremal Bell inequalities specifying the range of expectations of full correlation functions for any local realistic model.

The inequalities constructed in this way have a natural numbering, defined by the following procedure: For any number between 0 to $2^{2^n} - 1$, write the binary expansion with “digits” ± 1 to get f , and perform the inverse Fourier transform (9). From β compute the polynomial (3), which is often the best form of writing the inequality, because one can apply algebraic simplifications. For examples of this numbering, see the Appendix. The converse procedure is similar. For example, the MATHEMATICA package available from our website [12] finds that Mermin’s inequality for $n=6$ has the number 1 692 930 046 964 590 721.

C. Structure of the classical region

From the preceding section it is clear that the classical region Ω is a polytope in $d=2^n$ dimensions with $2d$ extreme points and 2^d maximal faces. This suggests that Ω should be a hyperoctahedron, whose polar \mathcal{B} is a hypercube. Indeed from the parametrization of the inequalities by d values $f(r) = \pm 1$, the latter statement is rather obvious. That Ω is an octahedron is not so apparent in the coordinates labeled by s as above. However, we can choose a basis transformation making this geometric identification of Ω more obvious. The necessary transformation is, of course, just the Fourier transform. With the notation

$$\hat{\xi}(r) = 2^{-n} \sum_s (-1)^{\langle r,s \rangle} \xi(s), \quad (10)$$

we can summarize the findings of the preceding section by saying that $\xi \in \Omega$ if and only if

$$\forall f \in \{-1,1\}^{2^n}: \sum_r f(r) \hat{\xi}(r) \leq 1. \quad (11)$$

The expression in Eq. (11) reaches its maximum with respect to f if $f(r)$ is just the sign of $\hat{\xi}(r)$. Therefore, the whole set of 2^{2^n} linear inequalities (or the statement $\xi \in \Omega$) is equivalent to the single nonlinear inequality

$$\sum_r |\hat{\xi}(r)| \leq 1. \quad (12)$$

Obviously, this nonlinear inequality is nothing but the characterization of the hyperoctahedron in 2^n dimensions as the unit sphere of the Banach space l^1 .

From this simple characterization of Ω it might seem that our problem is essentially trivial. However, the vast symmetry group of Ω , which includes among other transformations the set of $(2^n)!$ permutations of the coordinates is misleading, because these are not really symmetries of the underlying problem of finding all correlations within a classical model. This is apparent from the observation that the Bell polynomials associated with the extreme points may look quite different algebraically. That is, the 2^n dimensions are not really equivalent, but carry some structure coming from the division of the system into n sites. This is even more obvious when looking at the set of quantum correlations, which has a much lower symmetry. Nevertheless, the underlying problem has a large symmetry group, which will be studied in the next section.

IV. SYMMETRIES AND SUBSTITUTIONS

Browsing through the complete set of linear correlation inequalities one quickly gets the feeling that there are many rather similar ones, and also some inequalities which can be obtained in a rather trivial way (e.g., as a product) from lower-order ones. In this section we will describe the grouping of the inequalities into “essentially different ones,” and also how they can be obtained by an efficient construction for composing higher-order inequalities from lower-order ones. Both ways of structuring the set of inequalities make sense for more general cases (n,m,v) (see Sec. II), but for the moment we only apply them to our restricted class.

A. Symmetry group

Some symmetries acting on Bell inequalities are obvious and, in fact, present in any problem of this type, involving any number of outcomes and observables. The basic symmetries leading to equivalent inequalities are as follows.

- (i) Changing the labeling of the observables at each site.
- (ii) Changing the names of the outcomes of each observable.
- (iii) Permuting subsystems.

Since we have two observables per site, there are 2^n ways of swapping the labels of observables at each site. Swapping the ± 1 outcomes of an observable $A_k(s_k)$ at site k results in a sign in all correlation functions involving this observable. We have already utilized the fact that swapping both $A_k(0)$ and $A_k(1)$ only results in an overall sign, so it is enough to consider sign changes for $A_k(1)$ only. Clearly, there are 2^n such sign changes. Expressed in terms of the function f these transformations amount to

$$f(r) \mapsto (-1)^{\langle s_0, r \rangle} f(r + r_0), \quad (13)$$

where r, s_0, r_0 all lie in $\{0,1\}^n$, and r_0 and s_0 are the parameters describing the sign changes and observable swaps, respectively. Together with the global sign change and the $n!$ permutations we thus find the group G of symmetry transformations in our case to have the order

$$|G| = n! \cdot 2^{2n+1}. \tag{14}$$

The *orbit* of a given inequality is defined as the set of all the inequalities generated from it by symmetry transformations. The number of elements in an orbit is $|G|$, divided by the order of the group of symmetries leaving an element of the orbit invariant. The number of different orbits is the number of “essentially different” inequalities. Obviously, Eq. (14) is an upper bound on the number of elements in each orbit. Since the union of all orbits is the set of all inequalities, this leads to a lower bound on the number of essentially different inequalities.

Note that $|G|$ increases much more slowly than 2^{2^n} , the total number of extremal inequalities. Therefore, for large n the classification up to symmetry hardly reduces the number of cases. Explicitly, we find

n	Inequalities	$ G $	Orbits
2	16	64	2
3	256	768	5
4	65 536	12 288	39
5	4 294 967 296	245 760	$\geq 17\,476$

For n up to 4, the number of orbits was obtained explicitly. However, for $n \geq 5$ the lower bound on the number of orbits makes it clear that listing all essentially different inequalities is not going to be useful. More detailed results up to $n=4$ will be shown in the Appendix.

B. Generating new inequalities by substitution

A simple way of generating inequalities for higher n is to partition the n sites into two subsets of sizes n_1 and $n_2 = n - n_1$ and to take arbitrary Bell polynomials for n_1 and n_2 sites, appropriately rename the variables, and to multiply the two expressions. For example, the polynomial

$$\frac{1}{2}(a_1 b_1 + a_1 b_2 + a_2 b_1 - b_1 b_2) c_1 \tag{15}$$

is obtained by multiplying a CHSH polynomial for the first two sites with the trivial polynomial “ c_1 ” on the third [note that for the sake of clarity we have substituted $A_1(0), A_2(1)$ with a_1, b_2 , etc.]. It is clear that this gives an extremal Bell inequality for three sites.

This procedure can be generalized considerably by noting that the product operation corresponds to the trivial two-site Bell polynomial “ $a_1 b_1$,” but nothing restricts us to using a trivial expression here. So in general, consider a partition of the sites into K subsets of sizes n_k , $\sum_{k=1}^K n_k = n$. Then pick an extremal Bell polynomial for K sites, written out in variables $A_1(0), A_1(1), \dots, A_K(1)$. Now substitute for each $A_k(s_k)$ an extremal Bell polynomial for n_k sites. We claim that the resulting polynomial in n variables is an extremal Bell polynomial.

Indeed, if we substitute for each of the variables either $+1$ or -1 , we will get $A_k(s_k) = \pm 1$ for each k, s_k because

we substituted extremal Bell polynomials. But then the same argument on the level of K sites shows that the value will be ± 1 .

We will say that a Bell polynomial is *elementary* if it cannot be obtained by substitution from lower order polynomials. Obviously, if an inequality is elementary, so is its entire orbit. Clearly, the CHSH inequality is elementary. Moreover, it is known that it is a good tool for generating higher-order inequalities by substitution: one of the constructions [10,11] of the Mermin’s inequalities is based on this idea. But in view of the rapid increase of the double exponential one might think that there must be many more elementary inequalities. However, we have the following result.

Proposition. The CHSH inequality is the only elementary Bell inequality in the class we consider, i.e., all these inequalities for $n > 2$ can be constructed by successive substitutions into the CHSH inequality.

It is an interesting open problem, whether this statement holds for other families of Bell inequalities, e.g., the one tabulated in [13].

We start the proof on the level of vectors $f \in \{-1, 1\}^{2^n}$ parametrizing an arbitrary extremal Bell inequality for n sites. We decompose the system into a partition of $K=2$ subsets of size $n-1, 1$ and rewrite

$$f(\underbrace{r_1, \dots, r_{n-1}}_{\tilde{r}}, r_n) = f(\tilde{r}, 0) \delta_{r_n, 0} + f(\tilde{r}, 1) \delta_{r_n, 1}. \tag{16}$$

The respective coefficients $\beta(s)$ of the n -site inequality are then obtained via Fourier transformation according to Eq. (9), and we get

$$\begin{aligned} \beta(s) &= 2^{-n} \sum_r f(r) (-1)^{\langle r, s \rangle} \\ &= \frac{1}{2} \beta_0(\tilde{s}) \sum_{r_n} (-1)^{s_n r_n} \delta_{r_n, 0} + \frac{1}{2} \beta_1(\tilde{s}) \sum_{r_n} (-1)^{s_n r_n} \delta_{r_n, 1} \\ &= \frac{1}{2} [\beta_0(\tilde{s}) + (-1)^{s_n} \beta_1(\tilde{s})], \end{aligned} \tag{17}$$

where $\beta_k(\tilde{s})$ are coefficients for extremal Bell inequalities for $n-1$ sites. If we now add the respective observables $A_k(s_k)$ and write out the corresponding Bell polynomial

$$\begin{aligned} B &= \sum_s \beta(s) \prod_{k=1}^n A_k(s_k) \\ &= \frac{1}{2} B_0[A_n(0) + A_n(1)] + \frac{1}{2} B_1[A_n(0) - A_n(1)], \end{aligned} \tag{18}$$

we immediately see that this is just a CHSH polynomial, where the observables of one site have been substituted by Bell polynomials B_0 and B_1 for $n-1$ sites.

V. QUANTUM VIOLATIONS

Provided with a huge number of Bell-type inequalities we now go beyond the classical accessible region. The first

question to arise is of course whether or not and to what extent quantum systems can violate these inequalities. To answer this question we will first provide an effective variational method for computing the maximal quantum violations and show, that they are bounded by those obtained for Mermin's inequalities. In Secs. V A and V B we will then briefly discuss the structure of the underlying quantum domain, and prove that the generalized GHZ state maximally violates any of the correlation inequalities.

A. Obtaining the maximal violations

In order to compute the maximal quantum violation of any correlation inequality we have to vary over one density operator ρ on a tensor product of n factors, and two operators in each factor. Assuming all tensor factors to have dimension d , this means d^{2n} parameters for the density operator and $2nd^2$ for the observables. Hence the numerical solution of this variational problem is not feasible, except for the most trivial cases (and even impossible, because d is, in principle, a free parameter). Fortunately, however, it turns out that computing the overall maximum is much easier than computing the maximal violation for a fixed state: we will reduce the computation to a variational formula in just n variables.

First we have to recall some basic notions. In quantum mechanics expectations of ± 1 -valued observables are described by Hermitian operators $A_k(s_k)$ with spectrum in $[-1, +1]$. Since we are only interested in maximal correlations, we may as well take the observables extremal in the convex set of Hermitian operators with $-1 \leq A \leq 1$, i.e., we may assume the observables to be unitary and thus $A^2 = 1$.

The general form of a Bell inequality for an n -partite quantum system, which is characterized by a density operator ρ , is then

$$\text{tr}(\rho B) := \text{tr} \left[\rho \sum_s \beta(s) \otimes_{k=1}^n A_k(s_k) \right] \leq 1, \quad (19)$$

where we will refer to B as the *Bell operator*, which is just the quantum counterpart of the Bell polynomial defined in Eq. (3). Of course, every expectation value (19) larger than 1 is called a violation of Bell's inequality.

In order to derive the maximal quantum violation, which is nothing but the operator norm of the Bell operator, we first define another operator C by

$$C := B \otimes_{k=1}^n A_k(0) = \sum_s \beta(s) \otimes_{k=1}^n C_k^{s_k}, \quad (20)$$

where we have set $C_k = A_k(1)A_k(0)$ and $C_k^0 = 1$. Since the C_k are commuting unitary operators, all summands of C can be diagonalized simultaneously, and the eigenvectors of C are tensor products of eigenvectors of the C_k . Every eigenvalue γ of C is therefore of the form

$$\gamma = \sum_s \beta(s) \prod_{k=1}^n \gamma_k^{s_k}, \quad (21)$$

where γ_k is an eigenvalue of C_k . It is clear from the above remarks that C commutes with its adjoint, so $\|C\|$ is just the

modulus of the largest eigenvalue. Now we utilize the fact that $\|B^*B\| = \|C^*C\|$, i.e., $\|B\| = \|C\|$ and obtain

$$\|B\| = \sup_{\{\gamma_k\}} \left| \sum_s \beta(s) \prod_{k=1}^n \gamma_k^{s_k} \right|, \quad (22)$$

where each γ_k runs over the eigenvalues of $C_k = A_k(1)A_k(0)$. This formula allows us to compute the largest expectation $\text{tr}(\rho B)$ for fixed real coefficients β (coming from a Bell inequality or not) and a fixed choice of observables $A_k(s_k)$, but with ρ chosen without further constraints to maximize the expectation.

What we are now interested in is the maximum also with respect to the $A_k(s_k)$. Since formula (22) depends only on the eigenvalues γ_k this will be given by the same expression, but with γ_k running not just over the eigenvalues of a particular operator C_k but over all γ_k which can be eigenvalues of products of unitary and Hermitian operators. Since such a product is again unitary, we have $|\gamma_k| = 1$. Moreover, as is easily seen in 2×2 examples, this is the only constraint in any Hilbert space dimension (see also Sec. V D). Hence for any choice of real coefficients $\beta(s)$ and observables $-1 \leq A_k(s_k) \leq 1$, we have, as the best possible bound,

$$\text{tr} \left[\rho \sum_s \beta(s) \otimes_{k=1}^n A_k(s_k) \right] \leq \sup_{\{\gamma_k\}} \left| \sum_s \beta(s) \prod_{k=1}^n \gamma_k^{s_k} \right|, \quad (23)$$

where the supremum runs over all $\{\gamma_1, \dots, \gamma_n\}$ with $|\gamma_k| = 1$. Moreover, the bound does not change with Hilbert space dimension, as long as all factors are nontrivial. A more detailed discussion of quantum violations utilizing Eq. (22) for the special cases $n = 3, 4$ can be found in the Appendix.

B. Mermin's inequalities and the overall maximum

Asking for the overall maximal quantum violation we may additionally vary over the set of inequalities. In utilizing the result obtained in the preceding section, we are able to express the norm of a Bell operator in terms of lower-order Bell operators. Moreover, it suffices to consider qubit systems and we may therefore set $A_k(s_k) = \vec{a}_k(s_k) \vec{\sigma}$, where $\vec{\sigma}$ is the vector of Pauli matrices and $\vec{a}_k(s_k)$ is a normalized vector in \mathbb{R}^3 .

Squaring Eq. (18) this leads to

$$B^2 = \frac{B_0^2}{2} \otimes [1 + \vec{a}_n(0) \vec{a}_n(1)] + \frac{B_1^2}{2} \otimes [1 - \vec{a}_n(0) \vec{a}_n(1)] \\ + [B_0, B_1] \otimes \frac{i}{2} [\vec{a}_n(0) \times \vec{a}_n(1)] \vec{\sigma}. \quad (24)$$

Without loss of generality we now assume that $\|B_0\| \leq \|B_1\|$ and estimate by induction

$$\|B\|^2 = \|B^2\| \leq 2 \|B_1\|^2 \leq 2^{n-1}. \quad (25)$$

This bound is indeed saturated by the set of inequalities going back to Mermin [8–11], which thus provides the overall maximal quantum violation. In fact, we will show that the converse is also true, so that we have the following.

Proposition. The orbit corresponding to Mermin's inequality is the only one for which the maximal violation $2^{(n-1)/2}$ is attained.

Before we continue proving the claimed uniqueness, we emphasize, however, that this does not, in general, imply that for a fixed quantum state Mermin's inequality is more strongly violated than any other.

We begin our proof with noting that the maximal norm of the Bell operator in Eq. (24) requires orthogonality of the observables, such that the respective phases in Eq. (22) have to be $\pm i$. Without loss of generality we can thereby restrict to the case $+i$ since the remaining signs just correspond to a transformation between two inequalities of the same orbit according to Eq. (13). Hence, Eq. (22) leads to

$$\begin{aligned} \|B_{\max}\| &= 2^{-n} \left| \sum_{r,s} f_{\max}(r) \prod_{k=1}^n (-1)^{s_k r_k} i^{s_k} \right| \\ &= 2^{-n} \left| \sum_r f_{\max}(r) \prod_{k=1}^n [1 + i(-1)^{r_k}] \right| \\ &= 2^{-n/2} \left| \sum_r f_{\max}(r) \prod_{k=1}^n [e^{i(\pi/4)(1-2r_k)}] \right| \\ &= 2^{-n/2} \left| \sum_r f_{\max}(r) (-i) \sum_k r_k \right|. \end{aligned} \quad (26)$$

If we now want B_{\max} to saturate the bound in Eq. (25), then following Eq. (26) we are left with four possible choice for f_{\max} , like $f_{\max}(r)=1$ for $(-i)^{\sum_k r_k}=1, i$ and $f_{\max}(r)=-1$ otherwise. Since these four inequalities again belong to the same orbit, the correlation inequality leading to the overall maximal quantum violation is indeed uniquely determined (up to equivalence transformations within one orbit).

C. Structure of the quantum domain

In the same manner as we did for the classical case we may ask for the structure of the region in the space of correlations, which is accessible within the framework of quantum mechanics. One of the first to investigate this question in more detail apparently was Tsirelson [16,17], while studying quantum generalizations of Bell's inequalities.

Let us begin with defining the quantum counterpart of the classical accessible region Ω , introduced in Sec. II,

$$\mathcal{Q} := \{ \xi | \xi_s = \text{tr}[\rho \otimes_{k=1}^n A_k(s_k)] \} \subset \mathbb{R}^{2^n}, \quad (27)$$

where $\{A_k\}$ are suitable observables and ρ is a quantum state in arbitrary dimension. The structure of \mathcal{Q} is much more complicated than that of $\Omega \subset \mathcal{Q}$. In particular, it is not a polytope. Nevertheless, we can explicitly parametrize its extreme points. For the sake of completeness we will first prove convexity of \mathcal{Q} , although this follows closely the work of Tsirel'son [17].

Consider a convex combination of vectors in \mathcal{Q}

$$\sum_{\alpha} \lambda^{(\alpha)} \xi^{(\alpha)}, \quad \xi^{(\alpha)} \in \mathcal{Q} \quad (28)$$

and an associated Hilbert space

$$\mathcal{H} = \otimes_{k=1}^n \mathcal{H}_k = \otimes_k \oplus_{\alpha} \mathcal{H}_k^{(\alpha)} \cong \oplus_{\alpha_1 \dots \alpha_n} \otimes_k \mathcal{H}_k^{(\alpha_k)}. \quad (29)$$

Then with $\rho = \oplus_{\alpha} \lambda^{(\alpha)} \rho^{(\alpha)}$, which is a density operator acting on the "diagonal subspace"

$$\oplus_{\alpha} \otimes_k \mathcal{H}_k^{(\alpha)} \subset \mathcal{H}, \quad (30)$$

and $A_k(s_k) = \oplus_{\alpha} A_k^{(\alpha)}(s_k)$ we are given a state and observables such, that the convex combination in Eq. (28) is indeed a proper element of \mathcal{Q} . Hence, \mathcal{Q} is convex.

Now let us return to the result obtained in Sec. V B. Following Eq. (22) we can write the maximal quantum violation of an arbitrary inequality β as

$$\sup_{\gamma_0 \dots \gamma_n} \sum_s \beta(s) \text{Re} \left(\gamma_0 \prod_{k=1}^n \gamma_k^{s_k} \right) \quad (31)$$

$$= \sup_{\varphi_0 \dots \varphi_n} \sum_s \beta(s) \xi_s(\varphi_0, \dots, \varphi_n), \quad (32)$$

where we have set $\xi_s(\varphi_0, \dots, \varphi_n) = \cos(\varphi_0 + \sum_k \varphi_k s_k)$. Now by the bipolar theorem [20] the convex set \mathcal{Q} is just given by the convex hull of these vectors:

$$\mathcal{Q} = \text{co}\{ \xi(\varphi_0, \dots, \varphi_n) \}. \quad (33)$$

D. Generalized GHZ states

It is a well-known fact that the generalized GHZ state defined by

$$|\Psi_{GHZ}\rangle = \frac{1}{\sqrt{2}} (|00\dots 0\rangle + |11\dots 1\rangle) \quad (34)$$

maximally violates Mermin's inequalities [10]. Astonishingly this is also true for any other of the 2^{2^n} correlation inequalities.

Proposition. Any extreme point of the convex set of quantum correlation functions as defined in Eq. (27) is already obtained for the generalized GHZ state. In particular, this implies that GHZ states maximally violate any of the presented correlation inequalities.

We have to show that for any set of angles $\{\varphi_0, \dots, \varphi_n\}$ there are suitable observables such, that

$$\langle \Psi_{GHZ} | \otimes_{k=1}^n A_k(s_k) | \Psi_{GHZ} \rangle = \cos \left(\varphi_0 + \sum_k \varphi_k s_k \right). \quad (35)$$

Therefore we choose observables $A_k(s_k) = \vec{a}_k(s_k) \vec{\sigma}$ with

$$\begin{aligned} \vec{a}_k(0) &= (\cos \alpha, \sin \alpha, 0) \\ \vec{a}_k(1) &= [\cos(\varphi_k + \alpha), \sin(\varphi_k + \alpha), 0]. \end{aligned} \quad (36)$$

These observables simply swap the basis vectors providing them with an additional phase factor, i.e.,

$$\vec{a}_k(s_k) \vec{\sigma} |j\rangle = \exp[i(-1)^j(\alpha + \varphi_k s_k)] |j \oplus 1\rangle, \quad (37)$$

where $j=0,1$ and \oplus means addition modulo 2. Hence, for the left-hand side of Eq. (35) two terms occur, which are just complex conjugates of each other, and we get

$$\langle \Psi_{GHZ} | \otimes_{k=1}^n A_k(s_k) | \Psi_{GHZ} \rangle = \text{Re} \left\{ e^{ian} e^{i \sum_k \varphi_k s_k} \right\}, \quad (38)$$

so that it just remains to set $\alpha = \varphi_0/n$.

VI. STATES WITH POSITIVE PARTIAL TRANSPOSES

The violation of one of the inequalities, which can be derived from Eq. (9), is a rather physical entanglement criterion, since we can at least in principle decide it experimentally by measuring the respective correlations. However, the difficulty in doing so is the choice of the observables, and optimizing them for a fixed state leads in general to a very high dimensional variational problem. An entanglement criterion, which is in contrast easy to compute, is the *partial transpose* proposed by Peres in [22]. Before we settle the relationship between these two entanglement criteria, we will briefly recall some basic notions.

The *partial transpose* of an operator on a twofold tensor product of Hilbert spaces $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined by

$$\left(\sum_j C_j \otimes D_j \right)^{T_1} = \sum_j C_j^T \otimes D_j, \quad (39)$$

where C_j^T on the right-hand side is the ordinary transposition of matrices with respect to a fixed basis. The generalization of this definition to an n -fold tensor product is straight forward, and we will denote the transposition of all sites belonging to a set $\tau \subset \{1, \dots, n\}$ by the superscript T_τ .

Recall further that a state is called *separable* or *classically correlated* if it can be written as a convex combination of tensor product states—otherwise, it is called *entangled*. A necessary condition for separability, which also turned out to be sufficient in the case of two qubits [23], but not in general (cf. [24]), is the positivity of all partial transposes with respect to all subsystems. Moreover, there is a conjecture by Peres [19] that this might even imply the existence of a local realistic model. In [18] we showed that the set of inequalities going back to Mermin [8] is indeed fulfilled for states satisfying this positive partial transpose condition. In the following we will show that this implication is not due to a special property of these inequalities, but holds for any Bell-type inequality in Eq. (19), as long as we consider expectations of full n -site correlations. This leads to the main result of this section.

Proposition. Consider an n -partite quantum system, where each of the parties has the choice of two dichotomic observables to be measured. Assume further, that the partial transposes with respect to all subsystems of the corresponding density operator are again positive semidefinite operators. Then all the 2^n correlations can be described in the context of a local realistic model.

In particular, this implies that if a state is biseparable with respect to all partitions, all the inequalities are satisfied even if there exists no convex decomposition into n -fold product states. In order to prove this proposition and to derive an upper bound for the expectation of the Bell operator, we first apply the variance inequality to ρ^{T_τ} and B^{T_τ} ,

$$(\text{tr } \rho B)^2 = (\text{tr } \rho^{T_\tau} B^{T_\tau})^2 \leq \text{tr}[\rho^{T_\tau} (B^{T_\tau})^2] \leq \text{tr}\{\rho[(B^{T_\tau})^2]^{T_\tau}\}. \quad (40)$$

Since we suppose that $\rho^{T_\tau} \geq 0 \forall \tau$ this holds for any partial transposition, and we may take the average with respect to all subsets τ , and have therefore to estimate the expectation of the operator

$$\begin{aligned} & \frac{1}{2^n} \sum_{\tau} \sum_{s, s'} \beta(s) \beta(s') \otimes_{k \in \tau} A_k(s_k) A_k(s'_k) \otimes_{k \notin \tau} A_k(s'_k) A_k(s_k) \\ &= \sum_{s, s'} \beta(s) \beta(s') \otimes_{k=1}^n \frac{1}{2} \{A_k(s_k), A_k(s'_k)\}_+, \end{aligned} \quad (41)$$

where $\{\cdot, \cdot\}_+$ denotes the anticommutator. Note that in the first line of Eq. (41) we have rearranged the tensor product and made use of

$$[A_k(s'_k)^T A_k(s_k)^T]^T = A_k(s_k) A_k(s'_k). \quad (42)$$

Since $A^2 = \mathbb{1}$ and $s_k, s'_k \in \{0, 1\}$ only two different operators can arise in every tensor factor in Eq. (41): either

$2\{A_k(0), A_k(1)\}_+$ or the identity operator. These two obviously commute, and we can therefore simultaneously diagonalize all the summands. What remains to be done is to substantiate our intuition that “if everything commutes, then we are in the classical regime.” For this purpose note that eigenvalues of the operator (41) are of the form

$$\sum_{s, s'} \beta(s) \beta(s') \prod_{k=1}^n \begin{cases} \chi_k, & s_k \neq s'_k \\ 1, & s_k = s'_k \end{cases}, \quad (43)$$

for suitable $-1 \leq \chi_k \leq 1$. But since we can always find classical observables \mathcal{C} with correlations

$$\langle \mathcal{C}_k(0) \mathcal{C}_k(1) \rangle = \chi_k, \quad (44)$$

we are able to construct a system which is classical in the sense that it may be described in the context of classical probability theory, such that Eq. (43) is the expectation of the square of the respective Bell polynomial. However, due to the defining properties of the Bell inequalities, this is indeed bounded by unity, which proves our claim that all the considered Bell inequalities are satisfied for states having positive partial transposes with respect to all their subsystems.

VII. CONCLUSION

We provided two approaches for constructing the entire set of multipartite correlation Bell inequalities for two dichotomic observables per site: the Fourier transformation of a 2^n -digit binary number and nesting CHSH inequalities. This set of inequalities led us to a single nonlinear inequality, which detects the existence of a local classical model with respect to the considered correlations. We were able to simplify the variational problem of obtaining the maximal quantum violation of the linear correlation inequalities, in particular showing, that these are attained for generalized GHZ states, and proved, that “ppt states” satisfy all these 2^{2^n} inequalities.

One crucial assumption was that each site has the only choice of two dichotomic observables to be measured. Permitting more observables per site, more outcomes per observable, or even the choice of “not measuring,” i.e., includ-

ing restricted correlation functions, would lead to noncommuting terms, and most of the arguments would fail. So this is obviously a starting point for further investigations. In particular, one may think of applying the mechanism of substitution (Sec. IV) in order to derive new classes of Bell inequalities.

Another open question concerns the hierarchy of the inequalities with respect to their quantum violations. That is, if a given inequality is violated for a fixed quantum state, is there a set of inequivalent inequalities that have to be violated as well?

Finally, we want to mention that there is recent work by Scarani and Gisin [25] pointing out that there might be a close relation between the quantum violation of multipartite Bell inequalities and the security of n -partner quantum communication.

Note added. Recently a closely related paper [30] was posted by Zukowski and Brukner. They also study constraints on correlation functions and obtain the inequalities we presented in Sec. III.

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APPENDIX

Recently more and more attention has turned to tri- and four-partite states, especially to symmetric states as laboratories for multipartite entanglement (cf. [26–28]). Therefore we will provide the complete set of Bell inequalities for these cases in a more explicit form and additionally give the maximal quantum violations, which we have numerically [29] obtained utilizing the method presented in Sec. V.

1. Inequalities for three sites

For $n=3$ Eq. (9) leads to the five essentially different Bell polynomials [for the sake of legibility we again substitute $A_1(0), A_2(1)$ with a_1, b_2 etc.],

$$a_1 b_1 c_1, \tag{A1}$$

$$\frac{1}{4} \sum_{k,l,m} a_k b_l c_m - a_1 b_1 c_1, \tag{A2}$$

$$\frac{1}{2} [a_1(b_1 + b_2) + a_2(b_1 - b_2)] c_1, \tag{A3}$$

$$\frac{1}{2} [a_1 b_1 (c_1 + c_2) - a_2 b_2 (c_1 - c_2)], \tag{A4}$$

$$\frac{1}{2} (a_1 b_1 c_2 + a_1 b_2 c_1 + a_2 b_1 c_1 - a_2 b_2 c_2). \tag{A5}$$

Polynomials (A1) and (A3) are just trivial extensions of lower-order inequalities, and polynomial (A5) belongs to the set developed by Mermin [8]. The maximal quantum violations, the number of the first inequality of each of the five orbits, and the sizes of the respective orbits are stated in the following table:

Inequality	Orbit	Quantum violation	Polynomial
0	16	1	(A1)
1	128	5/3	(A2)
3	48	$\sqrt{2}$	(A3)
6	48	$\sqrt{2}$	(A4)
23	16	2	(A5)

2. Inequalities for four sites

For $n=4$ we just give the number of the first inequality of each of the 39 orbits, its size, and the respective maximal quantum violations. The index p labels orbits, including an element which is invariant under permutations of the subsystems, and f indicates factorizing Bell polynomials [like polynomials (A1) and (A3) for tripartite systems].

Inequality	Orbit	Quantum violation
$0_{p,f}$	32	1
1_p	512	1.843
3_f	1024	5/3
6	1536	5/3
7	3072	1.932
15_f	192	$\sqrt{2}$
22	2048	1.932
23	1024	$\sqrt{5}$
24	1024	2
25	6144	$\sqrt{3}$
27	3072	$\sqrt{3}$
30	3072	$\sqrt{3}$
60_f	384	$\sqrt{2}$
105	128	$\sqrt{2}$
278_p	256	$\sqrt{5}$
279_p	512	2.556
280	3072	2.139
281	1536	1.819
282	3072	1.819
283	6144	2.078
286	1536	2.078
287	1536	2.326
300	3072	2
301	6144	5/3
303	3072	1.819
317	3072	2
318	1536	2
319	2048	2.139
360	1024	2.326
363	1536	$\sqrt{3}$
367	1536	$\sqrt{3}$
383_p	256	2
831_f	128	2
854_f	96	2
857	384	$\sqrt{2}$
874	384	2
1632	96	$\sqrt{2}$
1647	192	2
6014_p	32	$2\sqrt{2}$

The number of the inequality representing the orbit of Mermin's inequality is 6014.

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