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Spectral decomposition of Bell operators for multiqubit systems

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The spectral decomposition of multipartite Bell operators for two dichotomic observables per site, as introduced by Werner and Wolf [Phys. Rev. A **64**, 032112 (2001)], is done. Implications on the characterization of Bell inequalities as criteria of entanglement are discussed. © *2007 American Institute of Physics.*
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I. INTRODUCTION

Bell correlation inequalities are being used as criteria to decide whether a given composite state is entangled or not. For 2-qubit systems, the preparation of pure entangled states is fully characterized by the violation of Bell's inequalities.[2] For multipartite (e.g., multiqubit) systems the structure of the state space with respect to entanglement is much richer and the full class of entangled states that can be characterized by the violation of Bell inequalities is not known. The present state of the theory of multipartite Bell inequalities in relation to entanglement properties is reviewed in Ref. 8.

The multipartite generalization of Bell's test deals with a system composed of n particles in an experimental arrangement that involves an observer for each particle. Independently of the rest, each observer decides on one of m observables to measure, obtaining one out of ℓ possible outcomes. Such a setup is referred to as the (n,m,ℓ) experiment. Experimental runs may be tuned up in one of m^n forms, and in each of its forms the outcome is one out of ℓ^n possible data instances. For each (n,m,ℓ) triple the complete set of independent Bell correlation inequalities is finite.

We restrict ourselves to the $(n,2,2)$ case of multiqubit systems for which the theory for the full correlation Bell inequalities had been developed by Werner and Wolf.[7] The complete set of independent full correlation inequalities for n-qubit systems is known,[7,9] and it has the cardinality 2^{2^n}. Particular examples, well known already, are the CHSH inequalities (by Clauser, Horne, Shimoney, and Holt)[1] for the 2-qubit system and its generalization to n qubits provided by Mermin in Ref. 3. Paradoxically, Mermin's inequality admits a violation factor that grows exponentially with n, the size of the qubit system.

The corresponding class $\{B_f : f \in \mathcal{S}_n\}$ of Bell operators for n-qubit systems introduced in Ref. 7 is complete and conveniently indexed by f in the set $\mathcal{S}_n := \{-1,1\}^{2^n}$. The observables, $A_k(0)$ and $A_k(1)$ per qubit $k \in \{1,\ldots,n\}$, involved in the specification of the Bell operators, depend on certain geometric parameters determined by the experimental setup and are assumed to satisfy the condition $A_k(s_k)^2 = \mathbb{1}$, $s_k = 0,1$. From now on Bell operators are understood to belong to the n-qubit class.

The aim of the present paper is to provide the spectral decomposition of all the Bell operators in the n-qubit class. Some of its implications in the characterization of the entanglement of pure n-qubit states are discussed. The spectral decomposition of Bell operators for n-qubit systems had been tackled by Scarani and Gisin[5] already. However, our approach allows us to provide formulas for important quantities such as the singular values of B_f and Mermin operators for every n.

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Equally important is the determination of the spectral radius of B_f, which is posed as a tractable variational problem. Its solution yields the entangled n-qubit states that realize the maximal violation that is admitted by B_f in the given geometry of the experimental setup.

The spectral decomposition of operator B_f proceeds in two steps. First, we derive a formula that expresses B_f^2 in terms of the 1-qubit commutators $(i/2)[A_k(0),A_k(1)]$, $k=1,\ldots,n$. A particular version of the formula, valid for "extremal" Bell operators, was derived in Ref. 6. Our result has the implications listed below.

(a) The eigenstates of B_f^2 are the product states $|w\rangle := |w_1\rangle \cdots |w_k\rangle \cdots |w_n\rangle$ ($w \in \{-1,1\}^n =: \mathcal{C}$) of the eigenstates $|w_k\rangle$ of the 1-qubit commutators, $w_k \in \{-1,1\}$. All eigenvalues of B_f^2 are doubly degenerate at least.

(b) The Bell operator B_f admits a violation of the corresponding Bell inequality *if and only if its spectral radius is greater than* 1. We show how the spectral radius may be determined by solving a tractable optimization problem [see item (d) below]. This characterization of B_f as a probe of entanglement is thus useful since the number of independent Bell inequalities grows exceedingly fast with n.

(c) A formula for the singular values $\lambda_f(w) \geq 0$ of B_f is obtained.

(d) The spectral radius $\bar{\lambda}_f$ of B_f is the maximal quantum violation factor of the corresponding Bell inequality, for given values of the geometric parameters of the experimental setup. The determination of $\bar{\lambda}_f$ and the corresponding eigenstates is posed as a variational problem, in much simpler terms than the one posed in Ref. 7.

(e) The singular values of B_f are found to satisfy the sum rule

$$\sum_{w \in \mathcal{C}} \lambda_f^2(w) = \dim(\mathcal{H}) = 2^n. \tag{1}$$

The total spectrum [Eq. (1)] is independent of f and of geometric parameters in the experimental setup. That is, it is the same for all n-qubit systems. Thus, the difference between tests shows up in the way the total spectrum is distributed among states. Extreme cases are a test with a spectrum equally distributed among all states and a test with a spectrum concentrated in just two Greenberger-Horne-Zeilinger (GHZ) states [Eq. (2)]. In the first case the sum rule [Eq. (1)] implies that $\lambda_f(w)=1$, and the test does not detect entanglement. In the second case, the sum rule [Eq. (1)] implies that the overall maximal violation factor $\Lambda_n := 2^{(n-1)/2}$ is admitted by the test.[7]

We say that an index vector f is *extremal* if B_f has an *optimal* geometry where its maximal violation factor $\bar{\lambda}_f$ coincides with the overall maximum Λ_n. An extremal test B_f in an optimal experimental setup, also called a Mermin test, "concentrates" the overall maximal factor of violation Λ_n in two entangled states. In this sense, we may say that Mermin's is the sharpest test of entanglement.

(f) The Mermin operator B_f, with spectral radius Λ_n, is characterized by either of the following two equivalent assertions:

(1) Vector f is extremal and $\|(i/2)[A_k(0),A_k(1)]\|=1$ for each qubit k.
(2) Only two eigenvalues of B_f are nonzero.

(g) A formula is given to compute the extremal vectors f for each n. We find that there are just four Mermin tests for each $(n,2,2)$ experiment, of which *only two are independent*, a very small number as compared with the total number 2^{2^n}, $n \geq 2$, of Bell operators. Besides, the corresponding Mermin inequalities are violated by only two of the eigenstates of B_f. This result confirms the remark made in Ref. 4 that Mermin's phenomenon is the exception, not the rule.

All Mermin operators are computed easily by using our formula. In Appendix B we provide examples for $n=2$, 3, and 4. For $n=2$ they are the CHSH operators,[1] and for $n=3$ Bell polynomials were derived in Ref. 7 already.

The second step in the spectral decomposition of B_f is to apply the following elementary results of linear algebra. The operator B_f^2 is positive; then, it has a unique positive square root, denoted by $|B_f|$. The relevant fact is that the product states, eigenstates of B_f^2, are eigenstates of $|B_f|$ too. The corresponding eigenvalues $\lambda(w)$ are the singular values of B_f. Then, the Bell operator decomposes into the product $B_f = S_f|B_f|$, where, in general, the operator S_f is an isometry. A direct calculation shows us that, up to a phase factor, for any B_f the operator S_f is just the exchange of *antipodal* product states (the antipode of state $|w\rangle$ is the state $|\tilde{w}\rangle$, where configuration $\tilde{w}$ has components $\tilde{w}_k = -w_k$). These considerations immediately yield the following result.

(h) All eigenstates of B_f are GHZ states

$$|w,\pm\rangle = \frac{1}{\sqrt{2}}(|w\rangle \pm e^{i\varphi_f(w)}|\tilde{w}\rangle) \tag{2}$$

with eigenvalues $\pm\lambda_f(w)$ and configuration $w \in \mathcal{C}/\sim$, the quotient set where antipodal configurations are equivalent. Every $\lambda_f(w) > 1$ is the violation factor of the Bell inequality corresponding to B_f that is attained by the corresponding GHZ states [Eq. (2)].

(i) The configuration w of the GHZ states detected in a Mermin test depends on the geometry [specified by the set of angles introduced in definition (7) below]. Actually, the condition on the commutators in statement (1) above is a condition on the geometry. It is not too restrictive and leaves room for 2^n different geometries. Every such geometry determines an antipodal pair $w - \tilde{w}$, and there are two geometries accepting a given pair. For example, in a CHSH setup there are four geometries that admit the maximal violation factor: two geometries "put" the violation factor on the pair $\tilde{1}1$-$1\tilde{1}$ and two other geometries put it on the pair 11-$\tilde{1}\tilde{1}$.

II. THE B_f^2 OPERATOR

Each $(n,2,2)$ experiment admits the set $\mathcal{S}_n := \{0,1\}^n$ of experimental setups. Corresponding to each experimental setup $s \in \mathcal{S}_n$, there is the full correlation function $\xi(s) = \langle \Pi_{k=1}^n A_k(s_k)\rangle$ which is considered to be the s coordinate of the 2^n-dimensional real vector ξ. In Ref. 7 it was shown that the local-realistic hypothesis bounds vector ξ to lay in the convex hull Ω of the finite collection of vectors $\{\pm X_r : r \in \{0,1\}^n\}$, with coordinates $X_r(s) = (-1)^{\langle r,s\rangle}$, where $\langle r,s\rangle := \Sigma_k r_k s_k$. The assertion is equivalent to say that $\langle \beta, \xi\rangle \leq 1$ for each vector $\beta \in \Omega^\circ$, the polar set of Ω. The set Ω° is a polytope too, and it has a finite set of extremal (in the sense of convexity) points $\hat{f}$. Thus, fulfilling condition $\xi \in \Omega$ is equivalent to satisfying condition $\langle \hat{f}, \xi\rangle \leq 1$ for every extremal point $\hat{f}$ of Ω°. Extremal vectors of Ω° were determined in Ref. 7 to be the Fourier transform, on the group $\mathcal{S}_n \equiv \mathbb{Z}_2^n$,

$$\hat{f}(s) = 2^{-n} \sum_{r \in \mathcal{S}_n} (-1)^{\langle r,s\rangle} f(r), \tag{3}$$

of each function $f : \mathcal{S}_n \to \{-1,1\}$.

In the quantum theoretical description the quantity

$$\langle \hat{f}, \xi\rangle = \sum_{s \in \mathcal{S}_n} \hat{f}(s) \left\langle \prod_{k=1}^n A_k(s_k) \right\rangle$$

is replaced by the quantum expectation value of the operator

$$B_f = \sum_{s \in \mathcal{S}_n} \hat{f}(s) \bigotimes_{k=1}^n A_k(s_k), \tag{4}$$

one for each $f \in \{-1,1\}^{2^n}$. The freedom of choosing observables makes B_f depend on geometric parameters of the experimental setup. Thus, every vector f represents, not one, but a class of Bell operators.

In Appendix A we show that the operator B_f^2 is given by the formula

$$B_f^2 = \mathbb{1} + \sum_{\substack{p\subset\{1,\ldots,n\}\\ \#p \text{ is even}}} C_p(f) \bigotimes_{k\in p} \frac{i}{2}[A_k(0),A_k(1)], \tag{5}$$

where the sum is over all nonempty subsets of points $p\subset\{1,\ldots,n\}$ of even cardinality. Coefficients $C_p(f)$ depend on geometric parameters, and they are $2^{n-1}-1$ in number. Everyone is bounded to lay in the interval $[-1,1]$,

$$|C_p(f)| \leq 1. \tag{6}$$

Formulas to calculate $C_p(f)$ are given in Appendix A. A further property of coefficients is that $C_p(-f)=C_p(f)$, as it should be, given that $B_f^2=B_{-f}^2$.

Equality in Eq. (6) holds for vectors f of Mermin tests. In Appendix B we show that $C_p(f)=1$ is the condition that defines the extremal vectors f. The condition is independent of geometric parameters. Bell operators [Eq. (4)] having vectors f that satisfy condition $C_p(f)=1$ are the extremal Bell operators considered in Ref. 6.

The spectral decomposition of the Bell operator B_f in Sec. IV follows from the simple spectral properties of operator B_f^2 in Eq. (5). For the moment, remark that each operator $(i/2)\times[A_k(0),A_k(1)]$ in Eq. (5) is Hermitian and lying in the ball $\|A\|\leq 1$. Thus, it can be represented in the form

$$\frac{i}{2}[A_k(0),A_k(1)] = \sin\theta_k Z_k, \quad \theta_k \in [-\pi/2,\pi/2], \tag{7}$$

where each Hermitian operator Z_k is traceless and maximal, $\|Z_k\|=1$. The obvious choice is to take $Z_k=\sigma_z$, the same at each site k. It amounts to taking $A_k(s_k)=\langle n_k(s_k),\sigma\rangle$ with unitary vector $n_k(s_k)=(\cos\varphi_k(s_k),\sin\varphi_k(s_k),0)$ lying on the $x-y$ plane of a local coordinate system such that $n_k(1)\times n_k(0)=(0,0,\sin\theta_k)$. The orthonormal set $\{|w_k\rangle : w_k=-1,1\}$ of eigenvectors of σ_z is adopted as the basis of the state space $\mathcal{H}_k=\mathbb{C}^2$. The set of configurations for the product basis of $\mathcal{H}=\mathbb{C}^{2\otimes n}$ is $\mathcal{C}=\{-1,1\}^n$.

For each configuration $w=w_1w_2\cdots w_n\in\mathcal{C}$ the product vector

$$|w\rangle = |w_1\rangle\otimes|w_2\rangle\cdots\otimes|w_n\rangle \tag{8}$$

is an eigenvector of B_f^2 with eigenvalue

$$\lambda_f^2(w) = 1 + \sum_{\substack{p\subset\{1,\ldots,n\}\\ \#p \text{ is even}}} C_p(f)\prod_{k\in p} w_k \sin\theta_k \geq 0. \tag{9}$$

The following symmetries of B_f^2 and its eigenvalues are apparent from Eqs. (5) and (9).

(s.1) B_f^2 is invariant under the exchange of observables $A_k(0)\leftrightarrow A_k(1)$ at all points k. That is, $\sin\theta_k\leftrightarrow -\sin\theta_k$, and there are at least two geometries that yield identical results.

(s.2) $\lambda_f^2(w)$ is invariant under the simultaneous exchange $A_k(0)\leftrightarrow A_k(1)$ and $w_k\leftrightarrow\tilde{w}_k$ at any site k.

(s.3) For antipodal configurations $\lambda_f(w)=\lambda_f(\tilde{w})$. That is, the eigenvalues of B_f^2 are at least doubly degenerate.

As a corollary of the foregoing results, degeneracy of an eigenvalue $\lambda>1$ of B_f^2 is a necessary and sufficient condition for the existence of a pure entangled state that violates the Bell inequality corresponding to B_f. Such a state $|\lambda\rangle$ is not separable by necessity.

Lemma 2.1: Assume $\lambda>1$ *is an eigenvalue of* B^2. *Then*, (I) *there exists* $|\lambda\rangle$ *such that* $|\langle\lambda|B|\lambda\rangle|>1$ *if and only if* (II) λ *is degenerate*.

Proof: (II⇒I). We are assuming that $\lambda^2 > 1$ is a degenerate eigenvalue of B^2. The eigenspace $\mathcal{H}_\lambda$ of B^2 is B invariant. The restriction $B|_{\mathcal{H}_\lambda}$ is Hermitian, and thus it has eigenvectors $|\beta\rangle \in \mathcal{H}_\lambda$ with eigenvalues β such that $|\beta| = \lambda > 1$. Then, statement (I) follows.

Sufficiency is proven by contradiction ($\neg$II⇒$\neg$I). We are assuming that $\lambda > 1$, and by hypothesis ($\neg$II) the eigenspace $\mathcal{H}_\lambda$ of B^2 has $\dim(\mathcal{H}_\lambda) = 1$ (the case of a zero dimension is trivial) and is spanned by the eigenvector $|\lambda\rangle$ of B_f^2. Since $\mathcal{H}_\lambda$ is B invariant, then $|\lambda\rangle$ is an eigenvector of B, too. The contradiction stems from the fact that the unique state $|\lambda\rangle \in \mathcal{H}_\lambda$ is a product vector [Eq. (8)] for some configuration $w \in \mathcal{C}$, and then statement (I) is violated by the only (separable) state $|w\rangle \in \mathcal{H}_\lambda$. □

Symmetry (s.3) and Lemma 2.1 provide us with the following characterization of Bell tests as probes of entanglement in a $(n,2,2)$ experiment: B_f detects entangled states *if and only if* B_f^2 has a spectral radius that is greater than 1.

Formula (5) for B_f^2 implies that the eigenvalues [Eq. (9)] satisfy the sum rule [Eq. (1)]. The value for the sum [Eq. (1)] is independent of any geometric parameter and of f. Results [Eqs. (9) and (1)] allow us to think of the spectral function λ_f^2 as a weight function on the configuration set $\mathcal{C}$ with full weight $\#\mathcal{C} = 2^n$. The same amount of total weight is available in every test B_f, independent of f and of the choice of observables. The difference between tests consists in the way they distribute the weight in the configuration set $\mathcal{C}$. A test that equally distributes the weight among all configurations does not probe the entanglement since $\lambda_f^2(w) = 1$ for each $w \in \mathcal{C}$. This happens when $[A_k(0), A_k(1)] = 0$ at every point k.

Measurement B_f is a good probe of entanglement if the total weight $\#\mathcal{C}$ is supported in as few configurations as possible. In Sec. III we will see that the extremal situation is when λ_f^2 concentrates all of the weight that is available, $\#\mathcal{C}$, on just two configurations. The spectral radius of B_f is $\bar{\lambda}_f := \max_w\{\lambda_f(w)\}$. After Eq. (9), the maximum is attained by a configuration $\bar{w}$ such that [for given $C_p(f)$ and $\sin\theta_k$] it maximizes the sum

$$\sum_{\substack{p \subset \{1,\ldots,n\} \\ \#p \text{ is even}}} x(p) \prod_{k\in p} w_k \quad \text{where } x(p) = C_p(f) \prod_{k \in p} \sin\theta_k \in [-1,1]. \tag{10}$$

That is, $\bar{\lambda}_f = \lambda_f(\bar{w})$. In the sum there are $2^{n-1}-1$ terms, so that (except for $n=2$) they cannot for arbitrary f be made all positive by choosing just the n signs w_k. An important exception is constituted by vectors f such that $C(f) = 1$. The condition $C_p(f) = 1$ defines f as an extremal vector. In Appendix B we show that the condition does not involve a choice of geometric parameters. Thus, for extremal f the maximum is attained by choosing the signs $\bar{w}_k = \mathrm{sgn}(\sin\theta_k)$. The spectral radius of B_f is given by

$$\bar{\lambda}_f = \Bigg(1 + \sum_{\substack{p \subset \{1,\ldots,n\} \\ \#p \text{ is even}}} \prod_{k \in p} |\sin\theta_k|\Bigg)^{1/2} \quad \text{for } f \text{ satisfying } C_p(f) = 1. \tag{11}$$

The case $n=2$ is outside the foregoing discussion. Applying formulas from Appendix A the only $C_p(f)$ coefficient is computed to be $C_{\{1,2\}}(f) = (f(01)f(10) - f(00)f(11))/2 \in \{-1,0,1\}$. The case $C_{\{1,2\}}(f) = 0$ is irrelevant. The other two cases yield the spectral radius $\bar{\lambda}_f = \sqrt{1 + |\sin\theta_1 \sin\theta_2|}$, which is greater than 1 in any nontrivial geometry.

Thus, the variational problem

$$\bar{\lambda}_f = \max_w \left| \sum_s \hat{f}(s) e^{i\Sigma_k w_k \varphi_k(s_k)} \right|$$

posed in Ref. 7 (see Sec. IV) can be restated in simpler terms as the problem of finding the configuration w that maximizes the sum in Eq. (10).

The maximum violation factor for the Bell inequality corresponding to vector f is the maximum $\Lambda_f := \max_\varphi \bar{\lambda}_f$ taken over all geometries. Finally, the overall maximum is $\Lambda_n := \max_f \Lambda_f$.

III. MERMIN TESTS

The maximal violation factor Λ_n taken over all vectors f and over all geometries in every $(n,2,2)$ Bell experiment was determined by Werner and Wolf.[7] Here, directly from Eq. (11), we see that it is

$$\Lambda_n = \left(1 + \sum_{m=1}^{\lfloor n/2 \rfloor} \binom{n}{2m} \right)^{1/2} = 2^{(n-1)/2}. \tag{12}$$

The maximal violation factor is attained for a test B_f with a vector $f \in \{-1,1\}^{2^n}$ such that $C_p(f) = 1$ and for a geometry such that

$$|\sin \theta_k| = \left\| \frac{i}{2}[A_k(0), A_k(1)] \right\| = 1.$$

Thus, test B_f in a $(n,2,2)$ experiment is a Mermin test, with spectral radius $\Lambda_n = 2^{(n-1)/2}$, *if and only if* $C_p(f) = 1$ and $\|(i/2)[A_k(0), A_k(1)]\| = 1$.

What tests in a $(n,2,2)$ experiment are extremal? In Appendix B we prove that a vector f that satisfies the condition

$$f(s)f(s+p) = (-1)^{\langle p,s \rangle + \#p/2} \tag{13}$$

is an extremal one with $C_p(f) = 1$. In Eq. (13), $s \in \mathcal{S}_n$ and the subset $p \subset \{1, \ldots, n\}$, of even cardinality, are represented by the vector $p \in \mathcal{S}_n$ with coordinate $p_k = 1$ if $k \in p$ and $p_k = 0$ otherwise. Remark that for any two subsets p and p' of even cardinality, the symmetric difference $p + p'$ (coordinatewise mod 2 addition) is also of even cardinality. It means that the collection $\mathcal{P}_n := \{p : \#p = \text{even}\}$ (when $0 \cdots 0$ is included) is a subgroup of $\mathcal{S}_n$ of order 2^{n-1}. So, the set of independent conditions [Eq. (13)] lay on the orbits of two experimental setups $s \in \mathcal{S}_n$. For example, $s = 0 \cdots 00$ and $s = 0 \cdots 01$. The sign of the coordinates of f may be assigned in just two ways to each orbit. Thus, there are just four extremal tests B_f in any $(n,2,2)$ experiment, of which only two are independent.

Extremal vectors f, for any number n of qubits, are computed easily by using formula (13). The corresponding Bell operators for $n=2$ (the CHSH operators[1]), $n=3$ (derived in Ref. 7), and $n=4$ are computed in Appendix B.

IV. ALL BELL EIGENSTATES ARE GHZ

The spectral decomposition of B_f^2 is simple enough as to base on it the corresponding decomposition of B_f. To proceed, note that B_f^2 is a positive operator and it has a unique positive square root, denoted by $|B_f|$. Operator $|B_f|$ has the same set $\{|w\rangle\}$ of eigenvectors as B_f^2, with eigenvalues $\lambda_f(w) \geq 0$. Experiment B_f is decomposed then into the product $B_f = S_f |B_f|$, where, in general, the operator S_f is an isometry. For the particular form of operator B_f in Eq. (4) a direct calculation shows us that $B_f|w\rangle = \beta_f(w)|\tilde{w}\rangle$, with

$$\beta_f(w) = \sum_s \hat{f}(s) e^{i\sum_k w_k \varphi_k(s_k)} \quad \text{and} \quad \lambda_f(w) = |\beta_f(w)|.$$

Note that $\beta_f(w)$ is obtained from Eq. (4) by doing the replacement $A_k(s_k) \to \exp(i w_k \varphi_k(s_k))$. Thus, up to a phase factor, S_f is the permutation,

$$S_f|w\rangle = |\bar{w}\rangle := e^{i\varphi_f(w)}|\tilde{w}\rangle, \tag{14}$$

where the phase factor, whenever $\lambda_f(w) > 0$, can be written as $e^{i\varphi_f(w)} = \beta_f(w)/\lambda_f(w)$. Furthermore, $S_f^2 = \mathbb{1}$. The properties of S_f are used in the following construction.

Let $\mathcal{H}_\lambda \subset \mathcal{H}$ be an eigenspace of B_f^2 corresponding to the eigenvalue λ^2. Consider a product state $|w\rangle \in \mathcal{H}_\lambda$. By Eq. (14), the vectors

$$B_f|w\rangle = \lambda|\bar{w}\rangle \quad \text{and} \quad B_f|\bar{w}\rangle = \lambda|w\rangle$$

are orthonormal and lay in $\mathcal{H}_\lambda$, too. It is, of course, necessary that $\dim(\mathcal{H}_\lambda) > 1$. The foregoing properties of S_k imply that $\dim(\mathcal{H}_\lambda) \geqslant 2$ and that the $2-$dimensional subspace $\text{span}\{|w\rangle, |\tilde{w}\rangle\} \subset \mathcal{H}_\lambda$ is S_f invariant. Thus, every eigenvector of any Bell operators B_f is an entangled state of the form

$$|w;\pm\rangle = \frac{1}{\sqrt{2}}(|w\rangle \pm |\bar{w}\rangle) \tag{15}$$

with eigenvalues $\pm\lambda = \pm\lambda_f(w)$. We call such a superposition of antipodal states GHZ. Any Bell test in a $(n,2,2)$ experiment is diagonal in the GHZ basis. The maximal violation factor for a Bell inequality is the spectral radius of B_f and is attained by the GHZ states [Eq. (15)] with a configuration w that makes the sum [Eq. (10)] acquire its maximal value.

All eigenvectors of B_f come in entangled pairs of the GHZ form [Eq. (15)], two such states for each $w \in \mathcal{C}/\sim$. This result holds for all Bell operators in the n-qubit class and constitutes the main Theorem in Ref. 5.

In the GHZ basis *all* $(n,2,2)$ Bell operators have the diagonal form

$$B_f = \sum_{w \in \mathcal{C}/\sim} \lambda_f(w)(|w;+\rangle\langle w;+| - |w;-\rangle\langle w;-|). \tag{16}$$

Gisin's theorem[2] for 2-qubit systems is a direct consequence of the spectral decomposition (16).

Let us assume that B_f is a Mermin operator that admits the maximal violation factor $\Lambda_n = 2^{(n-1)/2}$. Then, according to Lemma 2.1, the corresponding Bell inequality is violated if and only if there exists at least two eigenstates $|w\rangle$ and $|\tilde{w}\rangle$ of B_f^2 with eigenvalue $\lambda_f^2(w) = \lambda_f^2(\tilde{w}) = 2^{n-1}$. But two such states saturate the sum rule [Eq. (1)], and there cannot be any other eigenstate involved in the violation of the Bell inequality (just one state is not enough because eigenstates of B^2 are separable). Thus, in every Mermin test the spectrum λ_f^2 equally distributes the total weight $\#\mathcal{C}$ in just two configurations (no less, no more). That is, B_f is a Mermin test if two and only two of its eigenstates violate the corresponding Bell inequality.

Mermin tests are optimal probes of entanglement in that they are tunable as to detect any antipodal pair $w-\tilde{w}$ by choosing the sign of $\sin\theta_k = \pm 1$ such that $w_k \sin\theta_k = 1$. That is, an extremal test B_f concentrates all the spectral weight λ_f that is available in just two GHZ states of our choice: $|w;+\rangle$ and $|w;-\rangle$.

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APPENDIX A: PROOF OF EQUATIONS (5) and (6)

From definition (4) we have

$$B_f^2 = \sum_{s,s' \in \mathcal{S}_n} \hat{f}(s)\hat{f}(s') \bigotimes_{k=1}^{n} A_k(s_k)A_k(s'_k) = \sum_{s,s' \in \mathcal{S}_n} \hat{f}(s)\hat{f}(s')\mathcal{O}(s,s'), \tag{A1}$$

where

$$\mathcal{O}(s,s') = \mathrm{Sym}_{s,s'} \bigotimes_{k=1}^{n} (\Phi_k(s_k,s_k') + i\Gamma_k(s_k,s_k')) \tag{A2}$$

is the symmetric component of the tensor-product operator in Eq. (A1). That is $\mathcal{O}(s,s') = \mathcal{O}(s',s)$. In Eq. (A2) we have made use of the following definitions:

$$\Phi_k(s_k,s_k') \coloneqq \frac{1}{2}\{A_k(s_k),A_k(s_k')\} = \mathbb{1}\frac{1+(-1)^{s_k+s_k'}}{2} + \frac{1}{2}\{A_k(0),A_k(1)\}\frac{1-(-1)^{s_k+s_k'}}{2}$$

and

$$\Gamma_k(s_k,s_k') \coloneqq \frac{-i}{2}[A_k(s_k),A_k(s_k')] = \frac{(-1)^{s_k}-(-1)^{s_k'}}{2}\frac{i}{2}[A_k(1),A_k(0)],$$

The Hermitian operators $\Phi_k(s_k,s_k')$ and $\Gamma_k(s_k,s_k')$ are symmetric and antisymmetric, respectively, under the exchange $s_k \leftrightarrow s_k'$. Furthermore, under the assumption that $A_k(s_k)^2 = \mathbb{1}$, we have $[\Phi_k(s_k,s_k'),\Gamma_k(s_k,s_k')] = 0$. These properties allow us to write the symmetric operator [Eq. (A2)] in the following form:

$$\mathcal{O}(s,s') = \sum_{\substack{p\subset\{1,\ldots,n\}\\ \#p \text{ is even}}} \bigotimes_{k\in p^c} \Phi_k(s_k,s_k') \bigotimes_{k\in p} \Gamma_k(s_k,s_k'), \tag{A3}$$

where the sum is over subsets $p \subset \{0,\ldots,n\}$ of even cardinality, including $p=\emptyset$.

Substituting Eq. (A3) in Eq. (A1), we obtain

$$B_f^2 = \mathbb{1} + \sum_{\substack{p\subset\{1,\ldots,n\}\\ \#p \text{ is even}}} (-1)^{\#p/2} \sum_{s,s'\in\mathcal{S}_n} \hat{f}(s)\hat{f}(s') \bigotimes_{k\in p} \Gamma_k(s_k,s_k') \bigotimes_{\ell\in p^c} \Phi_\ell(s_\ell,s_\ell'), \tag{A4}$$

where the term $\mathbb{1}$ is the contribution from $p=\emptyset$ and the sum now runs over nonempty subsets. Considering in Eq. (A4) that $(1/2)\{A_k(0),A_k(1)\} = a_k\mathbb{1}$, with $a_k = \cos\theta_k$, we get formula (5) for B_f^2 with coefficients, at the moment, given by

$$C_p(f) = (-1)^{\#p/2}2^{-n}F_f(p), \tag{A5}$$

where

$$F_f(p) \coloneqq \sum_{s,s'\in\mathcal{S}_n} \hat{f}(s)\hat{f}(s') \prod_{k\in p} \gamma(s_k,s_k') \prod_{\ell\in p^c} \varphi_\ell(s_\ell,s_\ell'), \tag{A6}$$

$$\gamma(s_k,s_k') = (-1)^{s_k} - (-1)^{s_k'}, \tag{A7}$$

and

$$\varphi_k(s_k,s_k') = 1 + (-1)^{s_k+s_k'} + a_k(1-(-1)^{s_k+s_k'}). \tag{A8}$$

Using (A7), the first product in (A6) expands to

$$\prod_{k\in p}\gamma(s_k,s'_k)=\sum_{r\subset p}(-1)^{\#r}(-1)^{\Sigma_{k\in r}s'_k+\Sigma_{k\in r^c}s_k},\tag{A9}$$

where $r\cup r^c=p$ and $r\cap r^c=\varnothing$. By using Eq. (A8), the second product in Eq. (A6) expands to

$$\prod_{k\in p^c}\varphi_k(s_k,s'_k)=\sum_{q\subset p^c}(-1)^{\Sigma_{k\in q^c}(s_k+s'_k)}\prod_{k\in q}(1+a_k)\prod_{\ell\in q^c}(1-a_\ell),\tag{A10}$$

where $q\cup q^c=p^c$ and $q\cap q^c=\varnothing$. The result for $F_f(p)$ in Eq. (A6) with the products expanded is

$$F_f(p)=\sum_{q\subset p^c}\prod_{k\in q}(1+a_k)\prod_{\ell\in q^c}(1-a_\ell)\sum_{r\subset p}(-1)^{\#r}G(q,r),\tag{A11}$$

where

$$G(q,r)=\sum_{s,s'\in\mathcal{S}_n}\hat{f}(s)\hat{f}(s')(-1)^{\Sigma_{k\in(q\cup r^c)}s_k+\Sigma_{k\in(q\cup r)}s'_k}.\tag{A12}$$

For the following, it is convenient to denote subsets $q\subset\{1,\ldots,n\}$ by vectors $q\in\mathcal{S}_n$ such that $k\in q$ iff $q_k=1$ (we are abusing the notation but no confusion will arise). With this identification, $G(q,r)$ in Eq. (A12) is seen to be the product of two inverse Fourier transforms,

$$G(q,r)=f(q+\bar{r})f(q+r),\tag{A13}$$

where $q\cup r\leftrightarrow q+r$ (because $qr=0$) and $r+\bar{r}=p$. Formula (A13) shows us that

$$|G(q,r)|=1.\tag{A14}$$

We have everything to prove inequality (6) From Eqs. (A5) and (A11) we have

$$|C_p(f)|\leqslant 2^{-\#p^c}\sum_{q\subset p^c}\prod_{k\in q}(1+a_k)\prod_{\ell\in q^c}(1-a_\ell),$$

where we have made use of Eq. (A14) and the fact that $|a_k|\leqslant 1$. One proves by induction in $\#p^c$ that

$$\sum_{q\subset p^c}\prod_{k\in q}(1+a_k)\prod_{\ell\in q^c}(1-a_\ell)=2^{\#p^c},\tag{A15}$$

and inequality (6) follows. Our final answer for $C_p(f)$ consists of formulas (A5), (A11), and (A13).

APPENDIX B: EXAMPLES OF MERMIN TESTS

In Mermin tests geometric parameters are settled down to $\sin\theta_k=\pm1$. That is $a_k=0$. Using the results obtained in Appendix A, the value $\bar{C}_p(f)$ of the coefficient [Eq. (A5)] for $a_k=0$ is

$$\bar{C}_p(f)=(-1)^{\#p/2}2^{-n}\sum_{s\in\mathcal{S}_n}(-1)^{\langle p,s\rangle}f(s)f(s+p),\tag{B1}$$

for each nonempty subset $p\subset\{1,\ldots,n\}$ of even cardinality. It is readily seen that a vector f that satisfies condition (13) makes $\bar{C}_p(f)=1$. On the other hand, substituting Eq. (13) in formulas (A5), (A11), and (A13), we see that $C_p(f)=1$ for any geometry. Thus, for such a vector f the operator B_f corresponds to an extremal one.

Extremal vectors f for $n=2$, 3, and 4, and the corresponding Mermin operators, are computed in the following.

For $n=2$ we have $\mathcal{P}_2=\{11\}$, which corresponds to the only subset $p=\{1,2\}$, of even cardinality. The orbits of setups 00 and 01 for condition (13) are

$$f(00)=-f(11) \quad \text{and} \quad f(01)=f(10).$$

The choice $f(00)=f(01)=1$ produces the vector $f=(1,1,1,-1)$, with Fourier transform $\hat{f}=(1/2,1/2,1/2,-1/2)$, which is extremal, and corresponds to one of the CHSH operators.

For $n=3$ we have the collection $\mathcal{P}_3=\{011,101,110\}$ that produces the two orbits

$$f(000)=-f(011)=-f(101)=-f(110),$$

$$f(001)=f(010)=f(100)=-f(111). \tag{B2}$$

Two independent choices of sign in Eq. (B2) give the vectors

$$f_1=(1,\ 1,\ 1,\ -1,\ 1,\ -1,\ -1,\ -1),$$

$$f_2=(1,\ -1,\ -1,\ -1,\ -1,\ -1,\ -1,\ 1),$$

with Fourier transforms

$$\hat{f}_1=\frac{1}{2}(0,\ 1,\ 1,\ 0,\ 1,\ 0,\ 0,\ -1), \quad \hat{f}_2=\frac{1}{2}(-1,\ 0,\ 0,\ 1,\ 0,\ 1,\ 1,\ 0) \tag{B3}$$

and Bell operators

$$B_{f_1}=\frac{1}{2}(A_1(0)A_2(0)A_3(1)+A_1(0)A_2(1)A_3(0)+A_1(1)A_2(0)A_3(0)-A_1(1)A_2(1)A_3(1))$$

and

$$B_{f_2}=\frac{1}{2}(-A_1(0)A_2(0)A_3(0)+A_1(0)A_2(1)A_3(1)+A_1(1)A_2(0)A_3(1)+A_1(1)A_2(1)A_3(0)).$$

Luckily, for $n=3$ half of the coordinates of vectors $\hat{f}$ in Eq. (B3) vanish. Thus, half of the experimental setups are not involved in extremal tests B_f for (3,2,2) experiments. The same situation happens for $n=5$ qubits. Is it a lucky strike?

The last example is for $n=4$ with a collection of subsets of even cardinality $\mathcal{P}_4=\{1100,1010,1001,0110,0101,0011,1111\}$ that produces the orbits

$$f(0000)=-f(0011)=-f(0101)=-f(0110)=-f(1001)=-f(1010)=-f(1100)=f(1111)$$

and

$$f(0001)=f(0010)=f(0100)=-f(0111)=f(1000)=-f(1011)=-f(1101)=-f(1110).$$

The choice of sign $f(0000)=f(0001)=1$ in the orbits gives the extremal vector

$$f=(1,\ 1,\ 1,\ -1,\ 1,\ -1,\ -1,\ -1,\ 1,\ -1,\ -1,\ -1,\ -1,\ -1,\ -1,\ 1),$$

with Fourier transform

$$\hat{f}=\frac{1}{4}(1,\ -1,\ -1,\ -1,\ -1,\ -1,\ -1,\ 1,\ -1,\ -1,\ -1,\ 1,\ -1,\ 1,\ 1,\ 1) \tag{B4}$$

and a Bell operator with 16 products of four observables each. The reader may construct B_f himself by using Eq. (4) with the extremal vector [Eq. (B4)].

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