Bell's inequalities for states with positive partial transpose

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We study violations of *n*-particle Bell inequalities (as developed by Mermin and Klyshko) under the assumption that suitable partial transposes of the density operator are positive. If all transposes with respect to a partition of the system into p subsystems are positive, the best upper bound on the violation is $2^{(n-p)/2}$. In particular, if the partial transposes with respect to all subsystems are positive, the inequalities are satisfied. This is supporting evidence for a recent conjecture by Peres that positivity of partial transposes could be equivalent to the existence of local classical models.

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I. INTRODUCTION

One of the basic questions asked early in the development of quantum information theory was about the nature of entanglement. Extreme cases were always clear enough: a two qubit singlet state was the paradigm of the entangled state [1], whereas product states and mixtures thereof were obviously not, but merely ''classically correlated'' [2]. But in the wide range between it was hardly clear where a meaningful boundary between the entangled and the nonentangled could be drawn. Still today, some boundaries are not completely known, although, of course, general structural knowledge about entanglement has increased dramatically in the last few years. The present paper is devoted to settling the relationship between two entanglement properties discussed in the literature.

To fix ideas we will start by recalling some properties one might identify with ''entanglement'' and the known relations between them. For simplicity in this introduction, we will choose the setting of bipartite quantum systems, i.e., quantum systems whose Hilbert space is written as a tensor product $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$. Moreover, we consider finite dimensional spaces only, leaving the appropriate extensions to infinite dimensions to the reader. All properties listed refer to a density matrix ρ on this space. It turns out to be simpler to define the entanglement properties in terms of there negations, i.e., the various degrees of ''classicalness.''

(S) A state is called *separable* or ''classically correlated,'' if it can be written as a convex combination of tensor product states. Otherwise, it is simply called ''entangled.''

(B) Before 1990 perhaps the only mathematically sharp criteria for entanglement were the Bell inequalities in their Clauser-Horn-Shimony-Holt (CHSH) form [3]. A state is said to satisfy these *Bell inequalities* if, for any choice of operators A_i, A_i' on $\mathcal{H}_i$ $(i=1,2)$ with $-\mathbf{1}\leqslant A_i, A_i'\leqslant\mathbf{1}$, we have

$$\mathrm{tr}\,\rho[A_1\otimes(A_2+A_2')+A_1'\otimes(A_2-A_2')]\leqslant 2. \qquad (1)$$

It is easy to see that $(S)\Rightarrow(B)$.

(M) Bell's inequalities are traditionally derived from an assumption about the existence of local hidden variables. The same assumptions lead to an infinite hierarchy of correlation inequalities [4], and it seems natural to base a notion of entanglement not on an arbitrary choice of inequality (e.g., CHSH) from this hierarchy. So we say that ρ *admits a local classical model*, if it satisfies all inequalities from this hierarchy. Then $(S)\Rightarrow(M)\Rightarrow(B)$. It was shown in [2] that $(M)\not\Rightarrow(S)$, and this was perhaps the first indication that different types of entanglement might have to be distinguished.

(U) A key step for the development of entanglement theory was a paper by Popescu [5], showing that by suitable local filtering operations applied to maybe several copies of a given ρ, one could sometimes obtain a new state ρ' violating a Bell inequality, even though ρ admitted a local hidden variable model, and hence satisfied the full hierarchy of Bell inequalities. Let us call a state *undistillable*, if it is impossible to obtain from it a two-qubit state violating the CHSH inequality, by any process of local quantum operations (i.e., operations acting only on one subsystem), perhaps allowing classical communication and several copies of the state as an input. What Popescu showed was that $(M)\not\Rightarrow(U)$.

(P) The idea of distillation was later taken to much greater sophistication [6], and for a while the natural conjecture seemed to be not only that $(S)\Rightarrow(U)$ (which is trivial to see), but that these two should be equivalent. The counterexample was provided in [7]. These authors used a property (P), which had been proposed by Peres [8] as a necessary condition for separability [i.e., $(S)\Rightarrow(P)$], which turned out also to be sufficient in the qubit case [9]. This condition (P) is that ρ has *positive partial transpose*, i.e., ρ^{T_1} is a positive semidefinite operator. Here the partial transpose A^{T_1} of an operator A on $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$ is defined in terms of matrix elements with respect to some basis by

$$\langle kl|A^{T_1}|mn\rangle=\langle ml|A|kn\rangle. \qquad (2)$$

Equivalently,

$$\left(\sum_\alpha A_\alpha\otimes B_\alpha\right)^{T_1}=\sum_\alpha A_\alpha^T\otimes B_\alpha, \qquad (3)$$

where the superscript T stands for transposition in the given basis. It was shown that $(P)\Rightarrow(U)$, and the counterexample

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in [7] worked by establishing (U) and not-(S) in this example. States of this kind are now called *bound entangled*.

There are further interesting properties, like usefulness for teleportation [10], but the above are sufficient for explaining the problem addressed in this paper. To summarize, it is known that $(S)\Rightarrow(P)\Rightarrow(U)$ and $(S)\Rightarrow(M)\Rightarrow(B)$. For pure states all conditions are equivalent, and for systems of two qubits $(U)\Rightarrow(S)$, but $(M)\not\Rightarrow(S)$.

For multipartite systems, i.e., systems with Hilbert space $\mathcal{H}_1\otimes\mathcal{H}_2\otimes\cdots\otimes\mathcal{H}_n$, the properties $(S),(M),(U)$ immediately make sense. For (B) there may be several choices of inequalities following from (M). The inequalities we use in this paper are discussed in detail in the next section. Partial transposition (P) is an intrinsically bipartite concept. The strongest version of (P) in multipartite systems is the one we use below: the positivity of partial transposes with respect to every subsystem.

Then the implication chains $(S)\Rightarrow(P)\Rightarrow(U)$ and $(S)\Rightarrow(M)\Rightarrow(B)$ hold as in the bipartite case. However, no direct relations are known so far between these chains, even in the bipartite case. It seems likely that the violation of (B) is a fairly strong property, perhaps implying distillability. This certainly seems to be the intuition of Peres in [11], who conjectures that

$$(M)\Leftrightarrow(P). \tag{4}$$

We will refer to this statement as *Peres' conjecture*. It should be noted, however, that neither we nor Peres have given a sharp mathematical formulation, particularly of the way the model is required to cover not only one pair but also tensor products and distillation processes. Some such condition is certainly needed (and implicitly assumed by Peres), because otherwise the implication $(M)\Rightarrow(P)$ would already fail for two qubits [2]. It is not entirely clear from [11] how strongly Peres is committed to Eq. (4). We are not completely convinced. However, we do follow Peres' lead in seeing here an interesting line of inquiry. Indeed, the present paper is devoted to proving one special instance of the conjecture, namely, the implication $(P)\Rightarrow(B)$, for general multipartite systems, where (P) is taken as the positivity of *every* partial transpose, and (B) is taken as the *n* particle generalization of the CHSH inequality proposed by Mermin [12], and further developed by Ardehali [13], Belinskii and Klyshko [15], and others [14,16].

II. MERMIN'S GENERALIZATION OF THE CHSH INEQUALITIES

Like the CHSH inequalities, Mermin's *n*-party generalization refers to correlation experiments, in which each of the parties is given one subsystem of a larger system and has the choice of two ±1-valued observables to be measured on it. The expectations of such an observable are given in quantum mechanics by a Hermitian operator A with spectrum in $[-1,1]$, and with a choice of A_k,A_k' at site k the raw experimental data are the 2^n expectation values of the form $\mathrm{tr}(\rho A_1\otimes A_2'\otimes\cdots A_n)$ with all possible choices A_k vs A_k' at all the sites.

If we look only at a single site, the possible pairs of expectation values (with fixed A,A' but variable ρ) lie in a square. It will be very useful for the construction of the inequalities and the proof of our result to consider this square as a set in the complex plane: after a suitable linear transformation (a $\pi/4$ rotation and a dilation) we can take it as the square $\mathcal{S}$ with the corners ±1 and $\pm i$. The pair of expectation values of A and A' is thus replaced by the single complex number $\mathrm{tr}(\rho a)$, where

$$a=\tfrac{1}{2}[(A+A')+i(A'-A)] \tag{5}$$

$$=e^{-i\pi/4}(A+iA')/\sqrt{2}. \tag{6}$$

The idea of this transformation is that the square $\mathcal{S}$ has a special property: products of complex numbers $z_k\in\mathcal{S}$ lie again in $\mathcal{S}$. This is evident for the corners (they form a group) and follows for the full square by convex combination. Suppose now that $\rho=\otimes_{k=1}^n\rho_k$ is a product state. Then the operator $b=\otimes_{k=1}^n a_k$ has expectation $\mathrm{tr}(\rho b)=\prod_{k=1}^n\mathrm{tr}(\rho_k a_k)\in\mathcal{S}$. Since the expectation is linear in ρ, the same follows for any separable state, i.e., any convex combination of product states. The statement "$\mathrm{tr}(\rho b)\in\mathcal{S}$" is essentially *Mermin's inequality*, although not yet written as an inequality. Note that the argument given here implies also that this statement (written out in correlation expressions involving A_k,A_k') holds in any local classical model, because in a classical theory every pure state of a composite system is automatically a product, and hence every state is separable. Thus Mermin's inequality indeed belongs to the broad category of Bell's inequalities.

To write "$\mathrm{tr}(\rho b)\in\mathcal{S}$" as a bona fide set of inequalities, we just have to undo the transformation (5), i.e., we introduce operators B,B' such that Eq. (5) is satisfied with (b,B,B') substituted for (a,A,A'). The operators B,B' are usually called *Bell operators*, and Mermin's inequality simply becomes

$$|\mathrm{tr}(\rho B)|\leq 1 \quad \text{or} \quad |\mathrm{tr}(\rho B')|\leq 1. \tag{7}$$

Writing out B and B' explicitly in terms of tensor products of A_k,A_k' gives the usual CHSH inequality (1) for $n=2$, and becomes arbitrarily cumbersome for large *n*. It is also not helpful for our purpose. The above derivation also gets rid of the case distinction "*n* odd/even," which has troubled the early derivations. In fact, Mermin [12] first missed a factor $\sqrt{2}$ for even *n*, which was later obtained by Ardehali [13], who in turn missed the same factor for odd *n*. Inequalities equally sharp for even and odd *n* were established in [14] and [15].

III. VIOLATIONS OF MERMIN'S INEQUALITY IN QUANTUM MECHANICS

The idea of combining A,A' in the non-Hermitian operator a has a long tradition for the CHSH case [17]. Its power is not only in organizing the inequalities (only linear transformations among operators are needed for that purpose), but in the possibility of bringing in the noncommutative algebraic structure of quantum mechanics to analyze the possibility of violations in the quantum case. In this section we discuss these violations, at the same time building up the machinery needed in the proof of our result. We will need the following expressions:

$$a^*a=\tfrac{1}{2}(A^2+A'^2)+\frac{i}{2}[A,A'], \tag{8}$$

$$aa^*=\tfrac{1}{2}(A^2+A'^2)-\frac{i}{2}[A,A'], \tag{9}$$

$$a^2-a^{*2}=i(A'^2-A^2). \tag{10}$$

It is clear from the first line that although $\mathrm{tr}(\rho\, a)$ lies in $\mathcal{S}$, and hence in the unit circle for all ρ, the operator norm $\|a\|=\|a^*a\|^{1/2}$ may be greater than 1. Therefore, the tensor product operator b may have a norm increasing exponentially with n. This is the key to the quantum violations of Mermin's inequality.

The largest possible commutators, i.e., operators saturating the obvious bound $\|[A,A']\|\leqslant 2\|A\|\|A'\|$ are just Pauli matrices. A good choice is $A_k=(\sigma_x+\sigma_y)/\sqrt{2}$ and $A'_k=(\sigma_x-\sigma_y)/\sqrt{2}$ for all k. Then $a_k=\sqrt{2}v$, where $v=\left(\begin{smallmatrix}0&0\\1&0\end{smallmatrix}\right)$. It is readily verified that $v^{\otimes n}$ acts in the two-dimensional space spanned by $e_1^{\otimes n}$ and $e_2^{\otimes n}$ exactly as v acts in the space spanned by the two basis vectors $e_1,e_2\in\mathbb{C}^2$. With the same identification of two-dimensional subspaces $b=2^{n/2}v^{\otimes n}$ acts like $2^{(n-1)/2}a$, so the possible expectations $\mathrm{tr}(\rho\, b)$ with ρ supported in this subspace span the exponentially enlarged square $2^{(n-1)/2}\mathcal{S}$.

In order to show that $2^{(n-1)/2}$ is the maximal possible violation (in analogy with Cirel'son's bound [18] for the CHSH inequality), but also in preparation for the proof of our main result, it is useful to consider the following general technique for getting upper bounds on $\mathrm{tr}(\rho\, b)$. It has been used in the CHSH case by Landau [19], among others. Note first that $\mathrm{tr}(\rho\, B)$ and $\mathrm{tr}(\rho\, B')$ are affine functionals of each A_k or A'_k. Hence, if we maximize the expectations of Bell operators by varying some A_k or A'_k, keeping ρ fixed, we may as well take A_k extremal in the convex set of Hermitian operators with $-\mathbf{1}\leqslant A_k\leqslant\mathbf{1}$. That is to say, we may assume $A_k^2=A_k'^2=\mathbf{1}$ for all k. Taking tensor products of Eq. (8) and expanding the product we find

$$b^*b=\bigotimes_{k=1}^{n}\left(\mathbf{1}+\frac{i}{2}[A_k,A'_k]\right)$$

$$=\sum_{\beta}\bigotimes_{k\in\beta}\frac{i}{2}[A_k,A'_k], \tag{11}$$

where the sum is over all subsets $\beta\subset\{1,\ldots,n\}$, and only factors different from $\mathbf{1}$ are written in the tensor product. In particular, the term for $\beta=\varnothing$ is $\mathbf{1}$. For bb^* we get a similar sum with an additional factor $(-1)^{|\beta|}$, where $|\beta|$ denotes the cardinality of the set β. From Eq. (10) we find $a_k^2=a_k^{*2}$ and $b^2=b^{*2}$ by taking tensor products. Again by applying Eq. (10), to (b,B,B') this time, we find that $B^2=B'^2$. In fact, by adding Eqs. (8) and (9) and inserting Eq. (11), we get

$$B^2=B'^2=\tfrac{1}{2}(b^*b+bb^*)$$

$$=\sum_{\beta\ \mathrm{even}}\bigotimes_{k\in\beta}\frac{i}{2}[A_k,A'_k]. \tag{12}$$

By the variance inequality $|\mathrm{tr}(\rho\, B)|^2\leqslant\mathrm{tr}(\rho\, B^2)$, the expectation of the right hand side is an upper bound on the square of largest violation of Mermin's inequality. There are two immediate applications: since each term in the sum has norm at most 1, the norm of the sum is bounded by the number of terms, i.e., 2^{n-1}. This shows the analog of Cirel'son's inequality, i.e., that the violation discussed above is indeed maximal. The second application is to the case that all commutators vanish. Then only the term for $\beta=\varnothing$ survives, and there is no violation of the inequality. Our result to be stated and proved in the next section is a refinement of this idea.

IV. POSITIVE PARTIAL TRANSPOSES AND MAIN RESULT

We now apply the technique of the previous section to the partial transpose. More specifically, for any density operator ρ and any subset $\alpha\subset\{1,\ldots,n\}$, let ρ^{T_α} denote the partial transpose of all sites belonging to α. Suppose now that ρ^{T_α} is positive semidefinite and hence again a density matrix. Then we can apply the variance inequality to ρ^{T_α} and B^{T_α}, obtaining

$$(\mathrm{tr}\,\rho B)^2=(\mathrm{tr}\,\rho^{T_\alpha}B^{T_\alpha})^2\leqslant\mathrm{tr}[\rho^{T_\alpha}(B^{T_\alpha})^2]$$

$$\leqslant\mathrm{tr}\{\rho[(B^{T_\alpha})^2]^{T_\alpha}\}. \tag{13}$$

We note that $[A^T,A'^T]^T=-[A,A']$ and thus

$$[(B^{T_\alpha})^2]^{T_\alpha}=\sum_{\beta\ \mathrm{even}}(-1)^{|\alpha\cap\beta|}\bigotimes_{k\in\beta}\frac{i}{2}[A_k,A'_k]. \tag{14}$$

Note that it does not matter whether we transpose α or its complement.

Now consider a partition of $\{1,\ldots,n\}$ into p nonempty and disjoint subsets $\alpha_1,\ldots,\alpha_p$. Let us denote by $\mathcal{P}$ the collection of all unions of these basic sets together with the empty set, so that $\mathcal{P}$ has 2^p elements. We assume that $\rho^{T_\alpha}\geqslant 0$ for all $\alpha\in\mathcal{P}$. For $p=1$ this is no constraint at all, because the full transpose of ρ is always positive. At the other extreme, for $p=n$, this assumption means the positivity of every partial transpose.

We now take the expectation value of Eq. (14) and average over the 2^p resulting terms. The coefficient of the βth term then becomes

$$2^{-p}\sum_{\alpha\in\mathcal{P}}(-1)^{|\alpha\cap\beta|}=2^{-p}\prod_{m=1}^{p}[1+(-1)^{|\alpha_m\cap\beta|}], \tag{15}$$

which is proved by writing the sum over $\mathcal{P}$ as a sum over p two-valued variables, labeling the alternative "$\alpha_m\subset\alpha$ or

$\alpha_m \not\subset \alpha$,'' and using that the parity $(-1)^{|\alpha\cap\beta|}$ is the product of the parities corresponding to the α_m. Clearly, the expression (15) is 1 if and only if $|\alpha_m \cap \beta|$ is even for all m and zero otherwise. Let us call such sets β ''$\mathcal{P}$ even.'' There are

$$\prod_m 2^{|\alpha_m|-1} = 2^{n-p} \tag{16}$$

such sets. Hence we get the bound

$$(\mathrm{tr}\,\rho B)^2 \leqslant \sum_{\beta\ \mathcal{P}\ \mathrm{even}} \mathrm{tr}\left(\rho \bigotimes_{k\in\beta} \frac{i}{2}[A_k, A'_k]\right) \leqslant 2^{n-p}. \tag{17}$$

That this bound is optimal is evident by evaluating it on a tensor product of pure states maximally violating Mermin's inequality for each partition element α_m, i.e., states as discussed in Sec. III.

To summarize, we have established the best bound

$$|\mathrm{tr}(\rho B)| \leqslant 2^{(n-p)/2} \tag{18}$$

on violations of Mermin's inequalities, under the assumption that the partial transposes ρ^{T_α} are positive for all $\alpha \subset \{1, \ldots, n\}$ subordinated to a partition into p subsets. This includes three special cases: For $p=1$ it is the analog of Cirel'son's inequality, for $p=n$ it proves our claim that the inequalities are satisfied if, all partial transposes are positive, and for partitions of the form $\{1\}, \ldots, \{m\}, \{m+1, \ldots n\}$, we obtain the result of Gisin and Bechmann-Pasquinucci [16] using Mermin's inequalities to test for the number m of independent qubits.

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