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# Maximal Violation of Bell Inequalities for Mixed States

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We show that mixed states can produce maximal violations in the Bell inequality due to Clauser, Horne, Shimony, and Holt (CHSH). This follows from the degeneracy of the operator which is naturally associated with the Bell inequality (here called the Bell operator). We have calculated the form of *all* the eigenvalues for the generic CHSH Bell operator. Finally, we consider several examples which demonstrate the utility of studying the eigenvalues and eigenvectors of the Bell operator.

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The concept of local realism [1] is that physical systems may be described by local objective properties that are independent of observation. Bell [2] showed that the assumption of local realism had experimental consequences, and was not simply an appealing world view. In particular, local realism implies constraints on the statistics of two or more physically separated systems. These constraints, called Bell inequalities, can be violated by the statistical predictions of quantum mechanics. For a very broad class of Bell inequalities these statistical constraints may be written as a locally realistic bound $\beta_{\rm LR}$ on the expectation value of some Hermitian operator $\hat{\mathcal{B}}$ (which we call a "Bell" operator), i.e.,

$$\langle\hat{\mathcal{B}}\rangle \le \beta_{\rm LR} \,.$$

We say that quantum theory predicts a violation of this Bell inequality if for some state this expectation value exceeds the bound $\beta_{\rm LR}$. In the language of operators the largest violation will be given by the largest eigenvalue of this Bell operator; and further, the states which can produce this maximal violation will be either eigenstates with this largest eigenvalue, or perhaps mixtures of them if they are degenerate. In this paper we construct examples where maximal violation is given by such mixtures, and we demonstrate the utility of the language of eigenvalues and eigenstates for this class of Bell inequalities.

The most commonly discussed Bell inequality is the Clauser-Horne-Shimony-Holt (CHSH) inequality [3]:

$$-2 \le C(a,b) + C(a,b') + C(a',b) - C(a',b') \le 2 \,, \tag{1}$$

where $a$ and $a'$ are two-valued ($\pm1$) variables for the first system, and $b$ and $b'$ are similar variables for the second system. The function $C(a,b)$ represents the correlation between $a$ and $b$ for the two systems — quantum mechanically it is given by $\langle\hat{a}\hat{b}\rangle$ with $\hat{a}$ and $\hat{b}$, Hermitian operators on Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$ corresponding to $a$ and $b$, respectively. Because their eigenvalues must be $\pm1$ these observables satisfy

$$\hat{a}^2 = \hat{a}'^2 = \hat{b}^2 = \hat{b}'^2 = \hat{I} \,, \tag{2}$$

where $\hat{I}$ is the identity operator.

Cirel'son [4] first proved that the absolute value of the combination of correlation functions in Eq. (1) is bounded by $2\sqrt{2}$ for any quantum mechanical calculation, instead of the 2 predicted by local realism. This means that the eigenvalues for the Bell operator

$$\hat{\mathcal{B}}_{\rm CHSH} \equiv \hat{a}\left(\hat{b}+\hat{b}'\right) + \hat{a}'\left(\hat{b}-\hat{b}'\right)$$

are bounded in magnitude by $2\sqrt{2}$. In our notation the CHSH Bell inequality becomes $-2 \le \langle\hat{\mathcal{B}}_{\rm CHSH}\rangle \le 2$.

A straightforward application of Eq. (2) shows [5] that

$$\hat{\mathcal{B}}^2_{\rm CHSH} = 4\hat{I} - [\hat{a},\hat{a}'][\hat{b},\hat{b}'] \,. \tag{3}$$

The consequences of this equation are rather surprising. If we go to bases where these commutators are diagonal, so that

$$i[\hat{a},\hat{a}'] = {\rm diag}(c_1, c_2, \ldots, c_{D(a)}) \,,$$

$$i[\hat{b},\hat{b}'] = {\rm diag}(d_1, d_2, \ldots, d_{D(b)}) \,,$$

with $\mathrm{diag}(c_1, c_2, \ldots, c_{D(a)})$ representing the diagonal matrix with diagonal elements $c_1, c_2, \ldots, c_{D(a)}$, and $D(a)$ and $D(b)$ are the dimensions of Hilbert spaces $\mathcal{H}_a$ and $\mathcal{H}_b$, then the eigenvalues $\mu_{ij}$ of the *square* of the Bell operator $\hat{\mathcal{B}}^2_{\mathrm{CHSH}}$ are given by

$$\mu_{ij} = 4 + c_i d_j ,$$

with $i = 1, \ldots, D(a)$ and $j = 1, \ldots, D(b)$; similarly, the eigenvalues $\lambda_{ij}$ of the Bell operator $\hat{\mathcal{B}}_{\mathrm{CHSH}}$ are given by

$$\lambda_{ij} = \pm\sqrt{\mu_{ij}} = \pm\sqrt{4 + c_i d_j} . \tag{4}$$

Cirel'son's bound is just equivalent to limits on the products: $-4 \le c_i d_j \le 4$.

Consider the subspace of eigenvectors of $\hat{\mathcal{B}}^2_{\mathrm{CHSH}}$ with some given eigenvalue $\mu$. To be specific we choose these eigenvectors as the outer product of states from $\mathcal{H}_a$ and $\mathcal{H}_b$—the natural choice as $\hat{\mathcal{B}}^2_{\mathrm{CHSH}}$ is diagonal here. In what way are the eigenvectors and eigenvalues of $\hat{\mathcal{B}}_{\mathrm{CHSH}}$ within this subspace inherited from those of $\hat{\mathcal{B}}^2_{\mathrm{CHSH}}$? In general, the eigenvectors of $\hat{\mathcal{B}}_{\mathrm{CHSH}}$ are linear combinations of the original eigenvectors, they are "entangled" as opposed to product states, and their eigenvalues are $\lambda = \pm\sqrt{\mu}$. We now show that if these eigenvalues correspond to a violation of the CHSH Bell inequality (i.e., $|\lambda| > 2$), then *both* signs must appear, i.e., both $\lambda = +\sqrt{\mu}$ and $\lambda = -\sqrt{\mu}$ appear. Suppose, to the contrary, that only one sign appears among all the eigenvectors of $\hat{\mathcal{B}}_{\mathrm{CHSH}}$ with this given magnitude $\sqrt{\mu}$ ($> 2$). Since the entire subspace is degenerate we can choose these eigenvectors as the original product state eigenstates of $\hat{\mathcal{B}}^2_{\mathrm{CHSH}}$. However, this is impossible as product states cannot produce a violation; they allow the correlation functions to factor, i.e., $\langle\hat{a}\hat{b}\rangle = \langle\hat{a}\rangle\langle\hat{b}\rangle$. When both signs appear, however, we are no longer free to "untangle" the eigenstates of $\hat{\mathcal{B}}_{\mathrm{CHSH}}$. Interestingly, this appearance of both signs for the eigenvalues is only *necessary* for those eigenstates which could lead to a violation.

Equation (3) has other implications as well. If *either* of the commutators $[\hat{a}, \hat{a}']$ or $[\hat{b}, \hat{b}']$ is zero then the eigenvalues become just $\pm 2$, so the expectation value $\langle\hat{\mathcal{B}}_{\mathrm{CHSH}}\rangle$ is bounded by the locally realistic limits, i.e., the violation goes away. Further, if *both* commutators vanish then all eigenstates of this "classical" Bell operator can be chosen to be product states with perfect correlations (or perfect anticorrelations) for each of the four correlation functions $C(a,b)$, $C(a,b')$, $C(a',b)$, and $C(a',b')$, i.e., in the "classical limit" there "really are" locally objective properties for each particle. Finally, if *neither* commutator vanishes then, since the trace of the commutators is zero (i.e., $\sum_i c_i = \sum_i d_i = 0$), we must have some of the $c_i d_j > 0$, and the corresponding eigenvectors will produce violations. Thus, for any CHSH Bell inequality based on noncommuting observables for both systems it is always possible to construct a state which will yield a violation (though not necessarily maximal). We now consider a few examples.

To simplify our discussion for the first two examples we restrict our attention to cases where the Hilbert space dimensionalities are equal and even, i.e., $D(a) = D(b) = 2n$, and further, that the two-valued observables have a simple block-diagonal form in some bases in terms of the $2 \times 2$ Hermitian matrices $A_i$, $A_i'$, $B_i$, and $B_i'$ ($i = 1, \ldots, n$), i.e.,

$$\hat{a} = \mathrm{diag}(A_1, A_2, \ldots, A_n) ,$$

with the square of each block being the identity to satisfy Eq. (2), and similar expressions apply for $\hat{a}'$, $\hat{b}$ and $\hat{b}'$.

Example 1: We make the choices [6]

$$A_i = \sigma_x , \quad A_i' = \sigma_y ,$$
$$B_i = \tfrac{1}{\sqrt{2}}(\sigma_x + \sigma_y) , \quad B_i' = \tfrac{1}{\sqrt{2}}(\sigma_x - \sigma_y) , \tag{5}$$

in terms of the Pauli spin matrices. The Bell operator then takes the form

$$\begin{aligned}\hat{\mathcal{B}}_{\mathrm{CHSH}} &= \sqrt{2}\,\mathrm{diag}(\sigma_x, \ldots, \sigma_x)_a \otimes \mathrm{diag}(\sigma_x, \ldots, \sigma_x)_b + \sqrt{2}\,\mathrm{diag}(\sigma_y, \ldots, \sigma_y)_a \otimes \mathrm{diag}(\sigma_y, \ldots, \sigma_y)_b \\ &= \sqrt{2}\,\mathrm{diag}\,(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y, \ldots, \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y)_{a\otimes b} .\end{aligned} \tag{6}$$

The Bell operator is seen to be highly degenerate, having $n^2$ duplicates of the eigenvalues of $\sqrt{2}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y)$; in particular, the eigenvalues are $\lambda = +2\sqrt{2}$, 0, and $-2\sqrt{2}$ with multiplicities of 1/4, 1/2, and 1/4, respectively, of the $4n^2$ eigenstates of the operator in Eq. (6). The eigenstates are also easy to enumerate; if we label our chosen bases for $\mathcal{H}_a$ and $\mathcal{H}_b$ by the vectors

$$|1,\uparrow\rangle,\ |1,\downarrow\rangle,\ |2,\uparrow\rangle,\ |2,\downarrow\rangle, \ldots, |n,\uparrow\rangle,\ |n,\downarrow\rangle ,$$

then each vector will stay in a two-dimensional subspace if acted upon only by the block-diagonal observables. With the bases labeled in this way the eigenvectors of $\hat{\mathcal{B}}_{\mathrm{CHSH}}$ are

$$|\Phi_{ij}^{(\pm)}\rangle = \tfrac{1}{\sqrt{2}}\Big(|i,\uparrow\rangle_a \otimes |j,\uparrow\rangle_b \pm |i,\downarrow\rangle_a \otimes |j,\downarrow\rangle_b\Big) ,$$
$$|\Psi_{ij}^{(\pm)}\rangle = \tfrac{1}{\sqrt{2}}\Big(|i,\uparrow\rangle_a \otimes |j,\downarrow\rangle_b \pm |i,\downarrow\rangle_a \otimes |j,\uparrow\rangle_b\Big) ;$$

the eigenvalues for $|\Phi_{ij}^{(\pm)}\rangle$ are zero, and those for $|\Psi_{ij}^{(\pm)}\rangle$ are $\pm 2\sqrt{2}$, respectively. Clearly, any mixture of the $|\Psi_{ij}^{(+)}\rangle$ states will still yield a maximal violation of $+2\sqrt{2}$, similarly for mixtures of the $|\Psi_{ij}^{(-)}\rangle$ yielding a violation $-2\sqrt{2}$.

Example 2: We take $A_1$, $A_1'$, $B_1$, and $B_1'$ as given in Eq. (5), and all the rest as the $2 \times 2$ identity matrix $I$.

In this case the CHSH Bell operator becomes

$$\hat{\mathcal{B}}_{\rm CHSH} = {\rm diag}(\sigma_x, I, \ldots, I)_a \otimes {\rm diag}(\sqrt{2}\sigma_x, 2I, \ldots, 2I)_b + {\rm diag}(\sigma_y, I, \ldots, I)_a \otimes {\rm diag}(\sqrt{2}\sigma_y, 0, \ldots, 0)_b$$

$$= {\rm diag}\Big(\sqrt{2}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y), \underbrace{2\sigma_x \otimes I,}_{n-1 \text{ copies}} \underbrace{\sqrt{2} I \otimes (\sigma_x + \sigma_y), \underbrace{2I \otimes I,}_{n-1 \text{ copies}}}_{n-1 \text{ copies}}\Big)_{a\otimes b} .$$

The first four eigenvalues are 0, $-2\sqrt{2}$, $+2\sqrt{2}$, and 0, and the rest consist of only +2 and −2 with multiplicities $4n(n-1)$ and $4(n-1)$, respectively. Thus, in this case no mixture can yield a maximal violation.

Example 3: Finally, we consider the Bell inequality recently discussed by Mermin [7] for $n$ spin-$\frac{1}{2}$ particles which yields a violation increasing exponentially with $n$. The Bell operator associated with his scheme is given by

$$\hat{\mathcal{B}}_{\rm M} = \frac{1}{2i}\left(\prod_{j=1}^{n}(\sigma_x^j + i\sigma_y^j) - \prod_{j=1}^{n}(\sigma_x^j - i\sigma_y^j)\right)$$

$$= -i2^{n-1}\left(\prod_{j=1}^{n} s_+^j - \prod_{j=1}^{n} s_-^j\right) ,$$

where $s_+^j$ and $s_-^j$ are the raising and lowering operators for the $j$th particle. Using this notation we may summarize Mermin's Bell inequality as

$$-2^{n/2} \le \langle\hat{\mathcal{B}}_{\rm M}\rangle \le 2^{n/2} , \quad n \text{ even} ,$$

$$-2^{(n-1)/2} \le \langle\hat{\mathcal{B}}_{\rm M}\rangle \le 2^{(n-1)/2} , \quad n \text{ odd} .$$

By defining the projection operators $P_+^j \equiv s_+^j s_-^j$ and $P_-^j \equiv s_-^j s_+^j$ which project particle $j$ onto the positive and negative $z$ axes, respectively, we can easily see that

$$\hat{\mathcal{B}}_{\rm M}^2 = 2^{2(n-1)}\left(\prod_{j=1}^{n} P_+^j + \prod_{j=1}^{n} P_-^j\right) .$$

The eigenvalues of this squared Bell operator are easily found in this diagonal representation: There are two equal to $2^{2(n-1)}$ and all the rest are zero. The nonzero eigenvalues correspond to two eigenvectors of $\hat{\mathcal{B}}_{\rm M}$,

$$|\Psi^{(\pm)}\rangle = \tfrac{1}{\sqrt{2}}\Big(|\uparrow\uparrow\cdots\uparrow\rangle \pm i|\downarrow\downarrow\cdots\downarrow\rangle\Big) ;$$

$|\Psi^{(+)}\rangle$ with eigenvalue $+2^{n-1}$ and $|\Psi^{(-)}\rangle$ with eigenvalue $-2^{n-1}$. This enumeration of the eigenvalues of $\hat{\mathcal{B}}_{\rm M}$ shows that the maximal violation will be produced by the state $|\Psi^{(+)}\rangle$ studied by Mermin (and also by $|\Psi^{(-)}\rangle$).

We have shown that mixed states can produce maximal violations in the CHSH Bell inequality. We constructed an example of arbitrarily high Hilbert space dimensionality for which one-quarter of the Hilbert space forms a subspace of degenerate eigenstates of the Bell operator with eigenvalue $+2\sqrt{2}$, another quarter is degenerate with eigenvalue $-2\sqrt{2}$, and the remainder is degenerate with eigenvalue zero. We proved that the general structure of the CHSH Bell operator implies that each Bell inequality violating eigenvalue (i.e., having magnitude greater than 2) must come in both signs. Also for any CHSH Bell inequality based on noncommuting observables for both systems we can always construct a state which will produce a violation (though not necessarily maximal). Finally, we have shown that the recent Bell inequality discussed by Mermin attains maximal violation for just the state he discusses.

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