# Violating Bell's Inequality Beyond Cirel'son's Bound

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Cirel'son inequality states that the absolute value of the combination of quantum correlations appearing in the Clauser-Horne-Shimony-Holt (CHSH) inequality is bound by $2\sqrt{2}$. It is shown that the correlations of two qubits belonging to a three-qubit system can violate the CHSH inequality beyond $2\sqrt{2}$. Such a violation is not in conflict with Cirel'son's inequality because it is based on postselected systems. The maximum allowed violation of the CHSH inequality, 4, can be achieved using a Greenberger-Horne-Zeilinger state.

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Bell's theorem [1] has been described as "the most profound discovery of science" [2]. It states that, according to quantum mechanics, the value of a certain combination of correlations for experiments on two distant systems can be higher than the highest value allowed by any local-realistic theory of the type proposed by Einstein, Podolsky, and Rosen [3], in which local properties of a system determine the result of any experiment on that system. The most commonly discussed Bell inequality, the Clauser-Horne-Shimony-Holt (CHSH) inequality [4], states that in any local-realistic theory the absolute value of a combination of four correlations is bound by 2. Cirel'son's inequality [5] shows that the combination of *quantum* correlations appearing in the CHSH inequality is bound by $2\sqrt{2}$ (Cirel'son's bound). It is widely believed that "[q]uantum theory does not allow any stronger violation of the CHSH inequality than the one already achieved in Aspect's experiment [6] [$2\sqrt{2}$]" [7]. However, it has been shown that exceeding Cirel'son's bound is not forbidden by relativistic causality [8]. Therefore, an intriguing question is why the CHSH inequality is not violated *more*. Here it is shown that, for three-qubit systems (that is, systems composed by three two-level quantum particles), the correlation functions of *two* suitably postselected qubits violate the CHSH inequality beyond Cirel'son's bound and that this violation can even reach 4, the maximum value allowed by the definition of correlation.

To introduce the CHSH inequality, let us consider systems with two distant particles $i$ and $j$. Let $A$ and $a$ ($B$ and $b$) be physical observables taking values $-1$ or 1 referring to local experiments on particle $i$ ($j$). The correlation $C(A,B)$ of $A$ and $B$ is defined as

$$C(A,B) = P_{AB}(1,1) - P_{AB}(1,-1) - P_{AB}(-1,1) + P_{AB}(-1,-1), \quad (1)$$

where $P_{AB}(1,-1)$ denotes the joint probability of obtaining $A=1$ and $B=-1$ when $A$ and $B$ are measured. In any local-realistic theory, that is, in any theory in which local variables of particle $i$ ($j$) determine the results of local experiments on particle $i$ ($j$), the absolute value of a particular combination of correlations is bound by 2:

$$|C(A,B) - mC(A,b) - nC(a,B) - mnC(a,b)| \leq 2, \quad (2)$$

where $m$ and $n$ can be either $-1$ or 1. The CHSH inequality (2) holds for any local-realistic theory, whatever the values of $m$ and $n$ are, in the allowed set, $\{-1,1\}$.

The bound 2 in inequality (2) can easily be derived as follows: In a local-realistic theory, for any individual system, the observables $A$, $a$, $B$, and $b$ have predefined values $v_A$, $v_a$, $v_B$, and $v_b$, either $-1$ or 1. Therefore, for an individual system the combination of correlations appearing in (2) can be calculated as

$$v_B(v_A - nv_a) - mv_b(v_A + nv_a), \quad (3)$$

which is either $-2$ or 2, because one of the expressions between parentheses is necessarily zero and the other is either $-2$ or 2. Therefore, the absolute value of the corresponding averages is bound by 2, q.e.d.

For a two-particle system in a quantum pure state described by a vector $|\psi\rangle$, the quantum correlation of $A$ and $B$ is defined as

$$C_Q(A,B) = \langle\psi|\hat{A}\hat{B}|\psi\rangle, \quad (4)$$

where $\hat{A}$ and $\hat{B}$ are the self-adjoint operators which represent observables $A$ and $B$. For certain choices of $\hat{A}$, $\hat{a}$, $\hat{B}$, $\hat{b}$, and $|\psi\rangle$, quantum correlations violate the CHSH inequality [4]. Therefore, no local-realistic theory can reproduce the predictions of quantum mechanics [1].

Later on, Cirel'son [5] demonstrated that for a two-particle system the absolute value of the combination of *quantum* correlations equivalent to those appearing in the CHSH inequality (2) is bound by $2\sqrt{2}$,

$$|C_Q(A,B) - mC_Q(A,b) - nC_Q(a,B) - mnC_Q(a,b)| \leq 2\sqrt{2}. \quad (5)$$

Cirel'son's bound can easily be derived as follows [9]: Consider the operator with the same structure as the combination which appears in inequality (5),

$$\hat{C} = \hat{A}\hat{B} - m\hat{A}\hat{b} - n\hat{a}\hat{B} - mn\hat{a}\hat{b}. \quad (6)$$

If $\hat{A}^2 = \hat{a}^2 = \hat{B}^2 = \hat{b}^2 = \mathbf{I}$, where $\mathbf{I}$ is the identity operator,

  

$$\hat{C}^2 = 4\mathbf{I} - mn[\hat{A},\hat{a}][\hat{B},\hat{b}]. \quad (7)$$

Since for all $\hat{F}$ and $\hat{G}$ bounded operators,

$$\|[\hat{F},\hat{G}]\| \leq \|\hat{F}\hat{G}\| + \|\hat{G}\hat{F}\| \leq 2\|\hat{F}\|\,\|\hat{G}\|, \quad (8)$$

then $\|\hat{C}^2\| \leq 8$, or $\|\hat{C}\| \leq 2\sqrt{2}$, q.e.d.

Different derivations of this bound can be found in [10,11]. Violations of the CHSH inequality (2) by $2\sqrt{2}$ can be obtained with pure [4] or mixed states [10].

Popescu and Rohrlich [8] raised the question whether relativistic causality could restrict the violation of the CHSH inequality to $2\sqrt{2}$ instead of 4, which would be the maximum bound allowed if the four correlations in the CHSH inequality (2) were independent. They prove this conjecture false [8] by defining a contrived correlation function which satisfies relativistic causality while still violating the CHSH inequality by the maximum value 4.

Here I shall show that violations of the CHSH inequality beyond the $2\sqrt{2}$ bound can be naturally obtained using only the predictions of quantum mechanics. This does not entail a violation of Cirel'son's inequality but a violation of the CHSH inequality beyond Cirel'son's bound. To understand the difference, let us consider three identical brothers. Every morning each of them takes a bus in London. One goes to Aylesbury, one to Brighton, and the third to Cambridge. Two of them wear white coats and the other wears a black one. We are interested in the correlations between the experiments on two of them. Then, the first step is to define which two. One possibility is to choose those brothers arriving in Aylesbury and Brighton. Another possibility is to choose those wearing white coats, regardless of their destination. Both possibilities are legitimate in a theory in which both procedures used for selecting pairs are related to predefined properties. According to Einstein, Podolsky, and Rosen [3], a local system is assumed to have a predefined property if we can predict with certainty the value of that property from the results of experiments on distant systems. Therefore, for a local-realistic theory, both procedures described above for selecting pairs would be legitimate. If we are interested in the correlations between the experiments on the two brothers with white coats, we can see whether the coat of the brother arriving in Cambridge is black. If this is the case, we can legitimately conclude that the other two brothers wear white coats. However, in quantum mechanics it is not meaningful to assume that some physical observables have predefined values before the measurements are made. Therefore, such an inference is not permitted.

The key for the understanding of our approach is to realize that, in searching for violations of the CHSH inequality (which is derived assuming local realism, without any mention of quantum mechanics), one is not limited to studying only the correlations of systems prepared in a quantum state, as in Cirel'son's inequality, but rather that one can use the correlations predicted by quantum mechanics for different subsets of systems previously prepared in a quantum state. Therefore, one can use a procedure like the one described above for selecting pairs. However, one cannot do this if we are interested in violations of Cirelson's inequality, which is valid for systems prepared in a quantum state (without any further postselection).

The important point for physics is not whether a quantum state violates the CHSH inequality but rather whether the predictions of quantum mechanics violate the CHSH inequality and the extent of this violation. We will show that the correlations of a postselected subsystem of a three-qubit system prepared in a Greenberger-Horne-Zeilinger (GHZ) state [12–14] as described by quantum mechanics allow the maximum violation.

Let us consider systems of three distant qubits prepared in the GHZ state:

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|+++\rangle + |---\rangle), \quad (9)$$

where $+$ and $-$ denote, respectively, spin-up and spin-down in the $y$ direction. For each three-qubit system prepared in the state (9), let us denote as qubits $i$ and $j$ those giving the result $-1$ when measuring the spin in the $z$ direction on all three qubits; the third qubit will be denoted as $k$. If all three qubits give the result 1, qubits $i$ and $j$ could be any pair of them. Since no other combination of results is allowed for state (9), qubits $i$ and $j$ are well defined for every three-qubit system. Generally, qubits $i$ and $j$ will be in a different location for each three-qubit system. For instance, if we denote the three possible locations as 1, 2, and 3, in the first three-qubit system, qubits $i$ and $j$ could be in locations 1 and 2; in the second three-qubit system, they could be in locations 1 and 3, etc. However, we can force qubits $i$ and $j$ to be those in 1 and 2, just by measuring the spin in the $z$ direction on the qubit in 3 and then selecting only those events in which the result of this measurement is 1.

We are interested in the correlations between two observables $A$ and $a$ of qubit $i$ and two observables $B$ and $b$ of qubit $j$. In particular, let us choose $A = Z_i$, $a = X_i$, $B = Z_j$, and $b = X_j$, where $Z_q$ and $X_q$ are the spin of qubit $q$ along the $z$ and $x$ directions, respectively. The particular CHSH inequality (2) we are interested in is the one in which $m = n = x_k$, where $x_k$ is one of the possible results, $-1$ or 1 (although we do not know which one), of measuring $X_k$. With this choice we obtain the CHSH inequality:

$$|C(Z_i,Z_j) - x_k C(Z_i,X_j) - x_k C(X_i,Z_j) - C(X_i,X_j)| \leq 2, \quad (10)$$

which holds for any local-realistic theory, regardless of the particular value, either $-1$ or 1, of $x_k$. Now let us use quantum mechanics to calculate the four correlations appearing in (10). By the definition of qubits $i$ and $j$, and taking into account that state (9) is an eigenstate of the self-adjoint operator $\hat{Z}_i\hat{Z}_j\hat{Z}_k$ with eigenvalue 1, we obtain

$$C(Z_i,Z_j) = 1, \quad (11)$$

since the only possible results are $Z_i = Z_j = 1$ and $Z_i = Z_j = -1$. By taking into account that state (9) is an eigenstate of $\hat{Z}_i\hat{X}_j\hat{X}_k$ with eigenvalue $-1$, we obtain

$$C(Z_i, X_j) = -x_k\,, \tag{12}$$

since the only possible results are $Z_i = 1$, $X_j = -x_k$ and $Z_i = -1$, $X_j = x_k$. By taking into account that state (9) is an eigenstate of $\hat{X}_i\hat{Z}_j\hat{X}_k$ with eigenvalue $-1$, we obtain

$$C(X_i, Z_j) = -x_k\,, \tag{13}$$

since the only possible results are $X_i = x_k$, $Z_j = -1$ and $X_i = -x_k$, $Z_j = 1$. Finally, by the definition of qubit $k$ as the one in which $z_k = 1$, and taking into account that state (9) is an eigenstate of $\hat{X}_i\hat{X}_j\hat{Z}_k$ with eigenvalue $-1$, we obtain

$$C(X_i, X_j) = -1\,, \tag{14}$$

since the only possible results are $X_i = -X_j = 1$ and $X_i = -X_j = -1$. Therefore, the left-hand side of inequality (10) is 4, which is the *maximum* value allowed by the definition of correlation. Other choices of three-qubit entangled quantum states and observables lead to violations of the CHSH inequality in the $2\sqrt{2}$ to 4 range.

This result opens the possibility of using sources of quantum entangled states of three or more particles [15] to experimentally test [16] local realism using not only proofs of Bell's theorem without inequalities [12–14] or Bell inequalities involving correlations between three or more particles [17,18], but also the CHSH inequality (10).

However, it must be stressed that, since the correlations (12) and (13) between qubits $i$ and $j$ depend on qubit $k$, the experimental test cannot be simply a test on, for instance, those pairs arriving in locations 1 and 2 when a particular measurement on the qubit arriving in 3 gives a particular result, but, as we shall see below, it requires treating all three qubits in a completely symmetrical way.

On the other hand, in real experiments using three qubits, the experimental data consist of the number of coincidences (that is, of simultaneous detections by three detectors) $N_{ABC}(a,b,c)$ for various observables $A$, $B$, and $C$. This number is proportional to the corresponding joint probability, $P_{ABC}(a,b,c)$.

Therefore, in order to make inequality (10) useful for real experiments, we must first translate it into the language of joint probabilities and then we must show how the joint probabilities of qubits $i$ and $j$ are related to the probabilities of coincidences of qubits arriving in 1, 2, and 3.

For the first step, it is useful to note that, by assuming physical locality (that is, that the expected value of any local observable cannot be affected by anything done to a distant particle), the CHSH inequality (10) can be transformed into a more convenient experimental inequality [19,20]:

$$\begin{aligned} -1 \leq P_{Z_iZ_j}(-1,-1) - P_{Z_iX_j}(-1,-x_k) \\ - P_{X_iZ_j}(-x_k,-1) - P_{X_iX_j}(x_k,x_k) \leq 0\,. \end{aligned} \tag{15}$$

The bounds $l$ of inequalities (2) and (10) are transformed into the bounds $(l-2)/4$ of inequality (15). Therefore, the local-realistic bound in (15) is 0, Cirel'son's bound is $(\sqrt{2}-1)/2$, and the maximum value is $1/2$. For qubits $i$ and $j$ of a system in the state (9),

$$P_{Z_iZ_j}(-1,-1) = 3/4\,, \tag{16}$$

since, in the state (9), the four possible results satisfying $z_iz_jz_k = 1$ (where $z_i$ denotes the result of measuring $Z_i$, etc.) have probability $1/4$ and in three of them $-1$ appears twice;

$$P_{Z_iX_j}(-1,-x_k) = 0\,, \tag{17}$$

since, in the state (9), $z_ix_jx_k = -1$;

$$P_{X_iZ_j}(-x_k,-1) = 0\,, \tag{18}$$

since, in the state (9), $x_iz_jx_k = -1$;

$$P_{X_iX_j}(x_k,x_k) = 1/4\,, \tag{19}$$

since, in the state (9), both results $x_i = x_j = x_k = 1$ and $x_i = x_j = x_k = -1$ have probability $1/8$. Therefore, as expected, the maximum allowed violation of inequality (15) occurs for the same choices in which the maximum violation of the CHSH inequality (10) does.

The second step consists of showing how the four joint probabilities (16)–(19) are related to the probabilities of coincidences in an experiment with three spatial locations, 1, 2, and 3. As can easily be seen,

$$\begin{aligned} P_{Z_iZ_j}(-1,-1) = P_{Z_1Z_2Z_3}(1,-1,-1) + P_{Z_1Z_2Z_3}(-1,1,-1) \\ + P_{Z_1Z_2Z_3}(-1,-1,1) \\ + P_{Z_1Z_2Z_3}(-1,-1,-1)\,, \end{aligned} \tag{20}$$

where, in the state (9), the first three probabilities in the right-hand side of (20) are expected to be $1/4$ and the fourth is expected to be zero. On the other hand, $P_{Z_iX_j}(-1,-x_k)$ and $P_{X_iZ_j}(-x_k,-1)$ are both less than or equal to

$$\begin{aligned} P_{Z_1X_2X_3}(-1,1,-1) + P_{Z_1X_2X_3}(-1,-1,1) \\ + P_{X_1Z_2X_3}(1,-1,-1) + P_{X_1Z_2X_3}(-1,-1,1) \\ + P_{X_1X_2Z_3}(1,-1,-1) + P_{X_1X_2Z_3}(-1,1,-1)\,, \end{aligned} \tag{21}$$

where, in the state (9), the six probabilities in (21) are expected to be zero. Finally,

$$P_{X_iX_j}(x_k,x_k) = P_{X_1X_2X_3}(1,1,1) + P_{X_1X_2X_3}(-1,-1,-1)\,, \tag{22}$$

where, in the state (9), the two probabilities in the right-hand side of (22) are expected to be $1/8$.

The experimental data of previous tests using three-photon systems prepared in a GHZ state [16] or possible new experiments over large distances with spacelike separated randomly switched measurements [21] or with three-ion systems and almost-perfect detectors [22] could experimentally confirm this violation of local realism predicted by quantum mechanics.

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