Quantum Contextuality: Violating Bell Inequalities with Qubits

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Abstract Quantum theory generally does not predict the outcomes of individual measurements. We might be tempted to think that the individual outcomes are determined by **hidden variables** that quantum theory doesn't know about. This article uses simple examples with qubits to show that such a model would need to have a strange feature in order to reproduce quantum theory's predictions.

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1 Introduction

Quantum theory generally does not predict the outcomes of individual measurements. We might be tempted to think that the individual outcomes are determined by **hidden variables (HVs)** that quantum theory doesn't know about, but the HVs idea can't reproduce quantum theory's predictions unless the HVs have a strange feature. Namely, the HVs would need to be **contextual**: the values they assign to one observable must depend on which observables are being measured. Noncontextual hidden variables cannot reproduce quantum theory's predictions.[1,2,3] This conclusion can be reached in several different ways. This article describes a few of them.

In quantum theory, some observables are not compatible with each other: they can't be measured together without compromising the quality of the measurements. Even if an observable A is compatible with both B and C, the observables B and C are not necessarily compatible with each other. Mathematically, two observables are not compatible with each other if they are represented by operators that don't share any eigenvectors with each other.[4] Observables that are incompatible with each other in this sense can't all have values when they're not being measured (article 03431). This results highlighted in this article are all related to that basic fact.

[1]Article 70833 has a complementary theme: noncontextual hidden variables cannot reproduce all of the results of experiments.

[2]Cabello (2013) points out that all **Bell inequalities**, like the CHSH bound highlighted in section 7, are based on some form of noncontextuality. Bell inequalities are famously violated both in quantum theory and in experiments.

[3]The literature about this subject is vast, and different authors may use the same words with different nuances.

[4]Some of the things we call "observables" are represented by operators that don't have any eigenvalues at all (they have purely continuous spectra instead), but in that case they can't be perfectly measured even by themselves (article 03431).

2 Prerequisites

In quantum theory, observables are represented by operators on a Hilbert space.[5] Here is a quick review of a few basic definitions:

- Two operators A and B are said to **commute** with each other if $AB = BA$.

- The **adjoint** A^* of an operator A is defined by requiring that $\langle\alpha|A^*|\beta\rangle$ be equal to the complex conjugate of $\langle\beta|A|\alpha\rangle$ for all vectors $|\alpha\rangle$ and $|\beta\rangle$ in the Hilbert space.

- A **projection operator** P is self-adjoint ($P^* = P$) and equals its own square ($P^2 = P$).

In this article, *operator* means linear operator, and I denotes the identity operator.[6]

In quantum theory, each of the possible outcomes of a measurement is represented by a projection operator. We can think of an observable as a collection of projection operators, each representing one of the possible outcomes when that observable is measured. We can package these projection operators into a single self-adjoint operator, which is usually a more convenient way to represent the observable. This article uses both representations.

The first two examples (sections 6-9) both use a pair of qubits. Sections 3-5 explain what that means, starting with the concept of a von Neumann algebra generated by a given set of operators. Here's a quick review of that concept. Let $\mathcal{A}$ be any set of operators on a Hilbert space, and let $\mathcal{A}'$ denote the **commutant** of $\mathcal{A}$, which is the set of operators that commute with everything in $\mathcal{A}$. Iterating this gives the **double commutant** $\mathcal{A}'' \equiv (\mathcal{A}')'$. If $\mathcal{A}$ includes the adjoint of each operator in $\mathcal{A}$, then $\mathcal{A}''$ is a von Neumann algebra (article 74088) called the algebra **generated by** $\mathcal{A}$. It includes the identity operator I and all of the operators in $\mathcal{A}$, and it's self-contained with respect to linear combinations and products.

[5] Article 03431 introduces the core principles of quantum theory.

[6] Several other articles in this series write the identity operator as "1" instead.

3 What is a qubit?

If P and Q are projection operators satisfying

$$2(P-Q)^2 = I, \tag{1}$$

then the algebra $\{P,Q\}''$ generated by $\{P,Q\}$ is called a **qubit**.[7,8] This definition of *qubit* doesn't require any of the operators in $\{P,Q\}''$ to be observables.

Equation (1) implies that the operators

$$Z \equiv 2P - I \qquad\qquad X \equiv 2Q - I \tag{2}$$

satisfy[9]

$$Z^2 = I \qquad\qquad X^2 = I \qquad\qquad XZ = -ZX. \tag{3}$$

A qubit can also be defined as the algebra $\{X,Z\}''$ generated by two operators X and Z satisfying (3), because for any such X and Z, the operators P and Q defined implicitly by (2) satisfy (1). Operators X and Z satisfying these conditions are called **Pauli operators**.

Qubits exist in any even-dimensional[10] (or infinite-dimensional) Hilbert space over $\mathbb{C}$. To prove this, partition the Hilbert space into two equal-dimensional orthogonal subspaces. Let P be the projection onto one of those subspaces. The fact that P is a projection operator gives the first equation in (3) when Z is defined by the first equation in (2). Let X be the operator that swaps the two subspaces with each other. This implies the second equation in (3) and also implies $XPX = I - P$, which gives the last equation in (3).

[7] Pronounced "Q-bit"

[8] This article uses the standard notation $\{A,B,C,...\}$ for the set whose elements are $A,B,C,...$, so $\{P,Q\}$ is the set whose two elements are the two operators P and Q. Don't confuse this with the anticommutator of P and Q, which is typically also written $\{P,Q\}$.

[9] For any projection operators P and Q, the relationships (2) imply the first two of equations (3) and $XZ+ZX = 2-4(P-Q)^2$. Combine this with (1) to get the third equation in (3).

[10] It must be even-dimensional because equations (2)-(3) give $XPX = X(I+Z)X/2 = (I-Z)/2 = I-P$. This says that P and $I-P$ are related to each other by a unitary transformation (because X is self-adjoint and unitary), so they project onto equal-dimensional subspaces.

4 The symmetry of a qubit

The previous section showed how to construct a qubit in any even-dimensional Hilbert space. In the case of a two-dimensional Hilbert space, a qubit consists of *all* of the operators on the Hilbert space.[11] This can be proved by showing that if P and Q satisfy (1), then any operator that commutes with both P and Q is proportional to the identity operator.[12] This implies that the double commutant $\{P, Q\}''$ includes all operators, because everything commutes with the identity operator.

The definition in the preceding section implies that any two qubit algebras are isomorphic to each other. In particular, any qubit is isomorphic to the algebra of all operators on a two-dimensional Hilbert space.[13] This means that a qubit is very symmetric: in any Hilbert space, if P and Q are any two projection operators satisfying (1), then the unitary operators in $\{P, Q\}''$ form a group isomorphic to $U(2)$. All of the nontrivial projection operators in $\{P, Q\}''$ are related to each other by these unitary transformations, and applying these unitary transformations to any one nontrivial projection operator in $\{P, Q\}''$ gives all of the other nontrivial projection operators in $\{P, Q\}''$.

[11]In contrast, two projection operators cannot generate all of the operators on a 3-dimensional Hilbert space (page 386 in Halmos (1969)).

[12]To prove this, choose a basis in which P and Q have the matrix representations

$$P = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad\qquad Q = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}.$$

Any 2×2 matrix that commutes with P must be diagonal, and any diagonal matrix that commutes with Q must be proportional to the identity matrix.

[13]This is the origin of the name qu*bit*. Section 5 gives more context.

5 Independent qubits

Let $\{P_1, Q_1\}$ and $\{P_2, Q_2\}$ be two pairs of projection operators, each satisfying (1):

$$2(P_1 - Q_1)^2 = I \qquad\qquad 2(P_2 - Q_2)^2 = I.$$

If both of $\{P_1, Q_1\}$ commute with both of $\{P_2, Q_2\}$, then these two qubits are said to be **independent** of each other.[14] More generally, N qubits are called independent of each other if they all commute with each other.

Here's an easy example of N independent qubits. Choose some integer $N \geq 1$, and let b denote an N-digit binary number. Consider a 2^N-dimensional Hilbert space spanned by vectors $|b\rangle$, one for each N-digit binary number, satisfying

$$\langle b|b\rangle = 1 \qquad\qquad \langle b'|b\rangle = 0 \;\text{ if }\; b' \neq b.$$

Any other vector in the Hilbert space is a linear combination of these basis vectors $|b\rangle$ with complex coefficients. For each $n \in \{1, 2, ..., N\}$, define operators Z_n and X_n by

$$Z_n|b\rangle = \begin{cases} |b\rangle & \text{if the } n\text{th digit is 0} \\ -|b\rangle & \text{if the } n\text{th digit is 1} \end{cases}$$

and

$$X_n|b\rangle = |b_n\rangle$$

where b_n is obtained from b by flipping the nth digit (replacing $0 \leftrightarrow 1$). Each pair $\{X_n, Z_n\}$ defines a qubit because it satisfies the conditions (3), and all of these N qubits commute with each other.

[14] According to theorem 4.1 in Summers (2008), the commutativity condition implies that the algebra generated by $\{P_1, Q_1\}$ and $\{P_2, Q_2\}$ is isomorphic to the **tensor product** of the two qubit algebras. (This follows from theorem 4.1 because each qubit algebra is a **factor**: its intersection with its commutant contains only multiples of the identity operator.) This article doesn't use the tensor product formalism, partly because in quantum field theory, the algebra generated by two qubits is often part of a larger algebra of observables for which the tensor product formalism is not helpful.

6 The Peres-Mermin square

This section reviews one of the easiest ways to show that noncontextual hidden variables cannot reproduce quantum theory's predictions.

Start with a system of two mutually commuting qubits, $\{X, Z\}$ and $\{\tilde{X}, \tilde{Z}\}$, where X and Z satisfy the conditions (3) and similarly for $\tilde{X}, \tilde{Z}$. Consider this set of nine operators, arranged in an array to make the pattern clear:

$$\begin{array}{ccc} X & \tilde{X} & X\tilde{X} \\ \tilde{Z} & Z & Z\tilde{Z} \\ X\tilde{Z} & \tilde{X}Z & X\tilde{X}Z\tilde{Z} \end{array}$$

Suppose that all of these operators are observables.[15] Each of these nine observables two eigenvalues, $+1$ and -1, which we can use to label the two possible outcomes when the observable is measured. Let A, B, C be the three observables in any one row or in any one column. In each case, A, B, C commute with each other, so their measurements are compatible with each other. The product ABC is equal to 1 in each case except the last row, in which case it is equal to -1. In other words, quantum theory predicts that if we measure all three observables in any one column or any one row, then the product of the outcomes will be $+1$, except for the last row in which case the product of the outcomes will be -1.

To reproduce quantum theory's predictions using noncontextual hidden variables, we would need to be able to replace this array of observables with an array of ± 1s such that the product of the three numbers in any column or any row is $+1$, except for the last row in which the product would need to be -1. That's clearly impossible, so noncontextual hidden variables cannot reproduce quantum theory's predictions.

The same conclusion can be reached in several different ways. The preceding proof was published in Peres (1990), who attributed it to Mermin. The array of

[15] An **observable** is something that can be measured in a single measurement event.

nine operators shown above is called a **Peres-Mermin square**. The Peres-Mermin proof assumes that the Hilbert space has at least four dimensions.[16] The **Kochen-Specker theorem** proves it using a Hilbert space that is only three-dimensional,[17] and that's the smallest Hilbert space supporting such a theorem.[18]

The Peres-Mermin and Kochen-Specker results are both state-independent: they depend on the pattern of observables but not on how the physical system is prepared. Sections 7-9 review a different approach, one that does depend on how the physical system is prepared but that is relatively easy to test in experiments. It uses a pair of qubits, like the Peres-Mermin approach does, so the Hilbert space must be at least four-dimensional. Sections 11-13 review a state-dependent approach that only needs a three-dimensional Hilbert space.

[16]The number of dimensions of the Hilbert space should not be confused with the number of dimensions of space(time). Most models of quantum systems in three-dimensional space (or four-dimensional spacetime) use a Hilbert space with an enormous number of dimensions, typically infinitely many.

[17]For a concise version of the proof, see endnote 4 in Conway and Kochen (2006).

[18]To describe the measurements as physical processes would require a Hilbert space with an enormous number of dimensions, but this article is using what article 03431 calls the **artificial approach**, which doesn't try to describe measurement as a physical process within the model itself.

7 Review of the CHSH bound

Section 9 shows that quantum theory violates the **CHSH bound**. This is another way to demonstrate that noncontextual hidden variables cannot reproduce quantum theory's predictions. The predicted violations have been observed in many experiments (article 70833). This section briefly reviews the CHSH bound.

The simplest type of observable is a **dichotomic** observable, one whose measurement has only two possible outcomes. To express the CHSH bound, these outcomes are usually labeled $+1$ and -1.

Suppose we have four dichotomic observables, A, B, C, D. Suppose that we can measure either A or C, and at the same time we can also measure either B or D, maybe in a different location. If we measure A and B, we get two numbers, both with magnitude $|\pm 1| = 1$. We we multiply these two numbers together, the result is either $+1$ or -1. Let $\langle AB\rangle$ denote the value of this product, averaged over many trials. This average is a number between -1 and $+1$. Consider the quantity

$$\Omega \equiv \langle AB\rangle + \langle CB\rangle + \langle CD\rangle - \langle AD\rangle. \tag{4}$$

Article 70833 shows that if the measurement outcomes were determined by noncontextual hidden variables, then this quantity would satisfy the inequality

$$-2 \leq \Omega \leq 2. \tag{5}$$

This is called the **CHSH bound**. Section 9 shows that in quantum theory, the quantity (4) can be as large as $2\sqrt{2} \approx 2.8$.[19] This shows that noncontextual hidden variables cannot reproduce quantum theory's predictions.

[19]This agrees with the results of real experiments, some of which are cited in article 70833.

8 Violating the CHSH bound: preview

The goal is to construct four observables A, B, C, D and a state for which the CHSH bound (5) is violated. To do this, consider two mutually commuting qubits $\{X, Z\}$ and $\{\tilde{X}, \tilde{Z}\}$, where X and Z satisfy the conditions (3) and similarly for $\tilde{X}, \tilde{Z}$. The observables A and C belong to one qubit, and the observables B and D belong to the other qubit. Explicitly,

$$\begin{aligned} A &= Z(0) & B &= \tilde{Z}(\pi/8) \\ C &= Z(2\pi/8) & D &= \tilde{Z}(3\pi/8) \end{aligned} \tag{6}$$

with

$$\begin{aligned} Z(\theta) &\equiv \cos(2\theta)\, Z + \sin(2\theta)\, X \\ \tilde{Z}(\phi) &\equiv \cos(2\phi)\, \tilde{Z} + \sin(2\phi)\, \tilde{X}. \end{aligned} \tag{7}$$

Section 9 shows that for any given values of θ and ϕ, the observables $Z(\theta)$ and $\tilde{Z}(\phi)$ each have two eigenvalues, $+1$ and -1, which we can use to label the possible outcomes when these observables are measured. Section 9 also shows that we can choose a state in which the probabilities for the various possible combinations of outcomes are as shown in this table:

Outcomes	Probability
$+1$ and $+1$	$\frac{1}{2}\cos^2(\theta-\phi)$
-1 and -1	$\frac{1}{2}\cos^2(\theta-\phi)$
$+1$ and -1	$\frac{1}{2}\sin^2(\theta-\phi)$
-1 and $+1$	$\frac{1}{2}\sin^2(\theta-\phi)$

The rest of the analysis is in article 70833, which shows that this distribtion maximally violates the CHSH bound (5) when the angles are chosen as in (6).

9 Violating the CHSH bound: calculation

Choose fixed values of θ and ϕ, and define $Z(\theta)$ and $\tilde{Z}(\phi)$ as in the previous section. Define operators $P(\theta)$ and $\tilde{P}(\phi)$ implicitly by

$$\begin{aligned} Z(\theta) &= P(\theta) - \big(I - P(\theta)\big) \\ \tilde{Z}(\phi) &= \tilde{P}(\phi) - \big(I - \tilde{P}(\phi)\big). \end{aligned} \tag{8}$$

The fact that X and Z satisfy equations (3) implies

$$\big(Z(\theta)\big)^2 = I,$$

and similarly for $\tilde{Z}(\phi)$. This, in turn, implies that the operators $P(\theta)$ and $\tilde{P}(\phi)$ defined in (8) are projection operators. When the observable $Z(\theta)$ is measured, the possible outcomes are represented by the projection operators $P(\theta)$ and $I - P(\theta)$, with corresponding eigenvalues $+1$ and -1, respectively, and similarly for $\tilde{Z}(\phi)$.

In quantum theory, information about how the physical system was prepared for a given measurement is represented by a **state**, a normalized positive linear functional that takes any operator as its input and returns a complex number as its output, subject to the conditions given in article 77228. Let $\rho(\cdots)$ denote the state before the measurements. According to the general principles of quantum theory (article 03431), if two projection operators Q and Q' commute with each other, then the probability of obtaining the combination of outcomes Q, Q' when both observables are measured may be written in any of these equivalent forms:

$$\rho(Q|Q')\rho(Q') = \rho(Q'|Q)\rho(Q) = \rho(QQ')$$

with

$$\rho(\cdots|A) \equiv \frac{\rho(A^* \cdots A)}{\rho(A^*A)}.$$

The probabilities of the possible combinations of outcomes when the observables (8) are both measured are shown in this table:

Outcomes	Probability
+1 and +1	$\rho\big(P(\theta)\tilde{P}(\phi)\big)$
−1 and −1	$\rho\big(\big(I-P(\theta)\big)\big(I-\tilde{P}(\phi)\big)\big)$
+1 and −1	$\rho\big(P(\theta)\big(I-\tilde{P}(\phi)\big)\big)$
−1 and +1	$\rho\big(\big(I-P(\theta)\big)\tilde{P}(\phi)\big)$

If we choose the state $\rho(\cdots)$ so that

$$\rho\big(P(\theta)\tilde{P}(\phi)\big) = \frac{1}{2}\cos^2(\theta-\phi), \tag{9}$$

then the identities

$$I - P(\theta) = P(\theta+\pi/2)$$
$$I - \tilde{P}(\phi) = \tilde{P}(\phi+\pi/2)$$

imply that the probabilities tabulated above will reproduce the distribution that was shown in section 8.

To construct a state that satisfies the condition (9), define the projection operator

$$Q \equiv \frac{I + X\tilde{X}}{2}$$

and let $|0\rangle$ be any nonzero vector that satisfies

$$Z|0\rangle = \tilde{Z}|0\rangle = |0\rangle. \tag{10}$$

Then the state

$$\rho(\cdots) = \frac{\langle\psi|\cdots|\psi\rangle}{\langle\psi|\psi\rangle} \qquad\qquad |\psi\rangle \equiv Q|0\rangle \tag{11}$$

satisfies the condition (9). To prove this, use equations (7) and (8) to get

$$2P(\theta) = I + \sin(2\theta)X + \cos(2\theta)Z$$
$$2\tilde{P}(\phi) = I + \sin(2\phi)\tilde{X} + \cos(2\phi)\tilde{Z}. \tag{12}$$

Equations (10) combined with the algebraic properties of $X, Z, \tilde{X}, \tilde{Z}$ imply that the only terms in $P(\theta)\tilde{P}(\phi)$ that contribute to the left-hand side of (9) are the terms proportional to $X\tilde{X}$, $Z\tilde{Z}$, and I.[20] Together with the identities

$$\rho(X\tilde{X}) = \rho(Z\tilde{Z}) = \rho(I) = 1,$$

this gives

$$\begin{aligned} 4\rho\big(P(\theta)\tilde{P}(\phi)\big) &= 1 + \sin(2\theta)\sin(2\phi) + \cos(2\theta)\cos(2\phi) \\ &= 1 + \cos(2\theta - 2\phi) \\ &= 2\cos^2(\theta - \phi). \end{aligned}$$

Altogether, this shows that the state defined by (11) satisfies the condition (9).

[20] To see that terms with exactly one of Z or $\tilde{Z}$ don't contribute, use the fact that Q is a projection operator, together with the identities $QX = XQ$ and $QZ = Z(1-Q)$ and similarly for $\tilde{X}$ and $\tilde{Z}$. Then use $QXQ = (X+\tilde{X})/2$ and (10) to see that terms proportional to X or $\tilde{X}$ don't contribute.

10 A bound that quantum theory can't violate

The preceding sections showed that the CHSH bound is violated in quantum theory. This section reviews **Cirelson's bound**,[21] which gives the maximum degree to which the CHSH bound can be violated in quantum theory.[22]

Let A, B, C, D be four observables in quantum theory. Suppose that A and C each commute with B and D, and consider the operator

$$\Omega \equiv C(B+D) + A(B-D).$$

If $A^2 = B^2 = C^2 = D^2 = I$, then

$$\Omega^2 = 4 - [A,C][B,D]$$

with $[X,Y] \equiv XY - YX$. Let $\|O\|$ denote the norm of an operator O, whcih is the maximum value of $\rho(O)$ among all states ρ. Use the general identities

$$\big\|[F,G]\big\| \leq \|FG\| + \|GF\| \leq 2\|F\|\,\|G\|$$

to get

$$\big\|\Omega^2\big\| \leq 8,$$

which implies

$$\|\Omega\| \leq 2\sqrt{2}.$$

This implies

$$\big|\rho(\Omega)\big| \leq 2\sqrt{2},$$

for all states ρ, which is Cirelson's bound.

Contrast this with the CHSH bound (5). The CHSH bound is violated in quantum theory, but Cirelson's bound is not.

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[21] Cirelson (1980). The author's name is often transliterated as *Tsirelson*.

[22] The derivation shown here is also shown in Cabello (2002) and in section 2 of Maldacena (2015).

11 The pentagram inequality, first version

Section 7 reviewed the CHSH bound, which is satisfied in any theory of noncontextual hidden variables but not in quantum theory. This section reviews another bound with similar significance: it is satisfied in any theory of noncontextual hidden variables but not in quantum theory. The original authors called it the **pentagram inequality**.[23] Compared to the CHSH bound, this one is even easier to describe and analyze.

Let P_0, P_1, P_2, P_3, and P_4 denote five different properties that a given object could have. For convenience, use the convention that all indices are defined modulo 5, so that $P_5 \equiv P_0$, and $P_6 \equiv P_1$, and so on. Whenever a measurement of P_k is performed to determine whether the object has that property, the result is either 1 ("yes, it has that property") or 0 ("no, it does not have that property").

Suppose that we choose this set of properties so that when the object is prepared in an appropriate special state, measurements of P_k and P_{k+1} do not both yield the outcome $+1$ for any consecutive pair k and $k+1$. I'll call this the no-consecutive-ones constraint.

The noncontextual hidden variables idea would say that in any given trial, we could assign values 1 or 0 to each of the P_k. The no-consecutive-ones constraint then implies that the object cannot have more than two of the five properties (no more than two of the values can be 1), so $\sum_k P_k \leq 2$. Even if the object's properties vary randomly from one trial to the next, as long as they respect the no-consecutive-ones constraint in each individual trial, we can take the expectation value of the preceding inequality to get

$$\sum_k \langle P_k \rangle \leq 2. \tag{13}$$

This is one version of the pentagram inequality. The reason for the name *pentagram* will become clear in section 13.

[23]Klyachko *et al* (2007). It is also called the **KCBS inequality** (Cabello (2013)) in honor of the original authors.

12 The pentagram inequality, second version

Given five properties P_k whose possible values are 1 or 0, as in the previous section, we can define observables $A_k = 2P_k - I$ whose possible values are $+1$ or -1. Now consider the sum

$$\sum_k A_k A_{k+1},$$

and suppose again that noncontextual hidden variables were possible, so that we can simultaneously assign values ± 1 to all of the A_ks. Then the product of the five terms in this sum would have to be $+1$, because each observable A_k appears twice in the product and $A_k^2 = 1$. Since each term in the sum is ± 1 and the product of all five terms is $+1$, the number of terms equal to -1 must be even. Therefore, the smallest possible value of the sum is

$$+1 + 4(-1) = -3,$$

so we have the inequality $\sum_k A_k A_{k+1} \geq -3$. As before, we can take the expectation value to get

$$\sum_k \langle A_k A_{k+1} \rangle \geq -3. \tag{14}$$

This inequality is also called the pentagram inequality.[24] This version is more general, because it holds even if the no-consecutive-ones constraint $P_k P_{k+1} = 0$ doesn't hold. To see this, use $A_k = 2P_k - I$ to deduce that (14) is equivalent to

$$\sum_k \langle P_k \rangle \leq 2 + \sum_k \langle P_k P_{k+1} \rangle,$$

which implies (13) if the no-consecutive-ones constraint is imposed.

The next section considers a situation that respects the no-consecutive-ones constraint. In that case, a violation of (13) implies a violation of (14), so the analysis in the next section shows that quantum theory violates both versions of the pentagram inequality.

[24]Klyachko *et al* (2007)

13 Violating the pentagram inequality

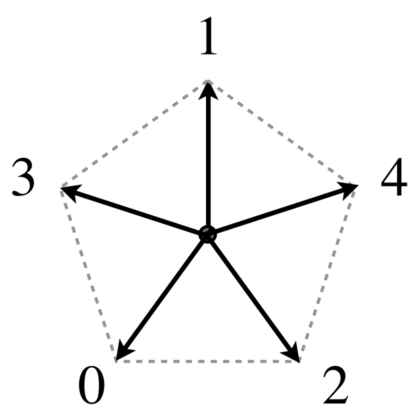
Both versions of the pentagram inequality are violated in quantum theory.[25] This section shows that in quantum theory, we can choose a set of five properties P_k (five projection operators) that satisfy $P_k P_{k+1} = 0$ for every k but which violate the pentagram inequality (13).

The construction uses a Hilbert space with only three dimensions. Within this Hilbert space, we will construct a set of five unit vectors $|k\rangle$, one for each $k \in \{0, 1, 2, 3, 4\}$, having the property that

$$\langle k|k+1\rangle = 0 \qquad\qquad \langle k|k\rangle = 1 \tag{15}$$

for all k. The index is defined modulo 5, so this condition implies $\langle 4|0\rangle = 0$.

We can contruct such a set of unit vectors with the help of some geometric intuition about ordinary unit vectors in ordinary three-dimensional space. Start with a regular pentagon, shown below as a dashed outline, and consider the five vectors pointing from the center of the pentagon to its vertices:



Label the vectors as shown in the picture,[26] so that the angle between vectors k and $k+1$ is $2\pi \times 2/5 = 4\pi/5$. In an orthonormal basis for ordinary 3d space, we

[25] Sadiq *et al* (2013) characterize the pentagram inequality as the "the simplest logical structure for which there is a classical-quantum gap."

[26] The name of the inequality comes from the fact that drawing lines to "connect the dots" in the order 0,1,2,3,4,0 gives a five-pointed star, also called a **pentagram**.

can take the components of these five vectors to be

$$\big(\cos(4k\pi/5),\, \sin(4k\pi/5),\, 0\big) \tag{16}$$

with $k \in \{0, 2, 3, 4, 5\}$. The angle between vectors k and $k+1$ is $4\pi/5$, so the dot product between them is

$$\cos(4\pi/5) = -\gamma \qquad\qquad \text{with } \gamma \equiv \cos(\pi/5) > 0. \tag{17}$$

Now, add the vector $(0, 0, \sqrt{\gamma})$ to each of the vectors (16) to get this new set of five vectors:

$$\big(\cos(4k\pi/5),\, \sin(4k\pi/5),\, \sqrt{\gamma}\,\big). \tag{18}$$

Use (17) to see that the dot product between vectors k and $k+1$ is now zero. The dot product of any one of these vectors with itself is $1+\gamma$.

Now let $|a\rangle$, $|b\rangle$, $|c\rangle$ be three orthogonal unit vectors in the Hilbert space. The intuition in the previous paragraph shows that the five vectors

$$|k\rangle \equiv \frac{\cos(4k\pi/5)\,|a\rangle + \sin(4k\pi/5)\,|b\rangle + \sqrt{\gamma}\,|c\rangle}{\sqrt{1+\gamma}} \tag{19}$$

satisfy the conditions (15). We can use these vectors $|k\rangle$ to show that quantum theory violates the pentagram inequality. Let P_k be the operator that projects onto $|k\rangle$, so that $\langle\psi|P_k|\psi\rangle = \langle\psi|k\rangle\langle k|\psi\rangle$ for any vector $|\psi\rangle$. The condition (15) implies $P_k P_{k+1} = 0$ for all k-modulo-5, so we can take these five projection operators to represent the "five properties" in section 11. To violate the pentagram inequality, consider the state

$$\rho(\cdots) = \frac{\langle c|\cdots|c\rangle}{\langle c|c\rangle}.$$

Equation (19) gives

$$\sum_k \rho(P_k) = \frac{\langle c|k\rangle\,\langle k|c\rangle}{\langle c|c\rangle} = \frac{5\gamma}{1+\gamma}. \tag{20}$$

To see that this violates the pentagram inequality (13), let's express the value of γ in a more explicit way. Use the identities

$$(e^{i\pi/5})^3 = -(e^{-i\pi/5})^2 \qquad\qquad e^{\pm i\pi/5} = \cos(\pi/5) \pm i\sin(\pi/5)$$

to get

$$\Big(\cos(\pi/5) + i\sin(\pi/5)\Big)^3 = -\Big(\cos(\pi/5) - i\sin(\pi/5)\Big)^2.$$

Take the imaginary part of this identity and cancel the overall factor of $\sin(\pi/5)$ to get

$$3\cos^2(\pi/5) - \sin^2(\pi/5) = 2\cos(\pi/5).$$

Write $\sin^2$ in terms of $\cos^2$ to get a quadratic equation for $\cos^2(\pi/5)$, whose positive solution is

$$\gamma \equiv \cos(\pi/5) = \frac{1+\sqrt{5}}{4}.$$

Use this in (20) to get

$$\sum_k \rho(P_k) = \sqrt{5} \approx 2.236 > 2,$$

which violates the pentagram inequality (13). The projection operators used in this construction satisfy the no-consecutive-ones constraint, so this shows that quantum theory also violates the more general inequality (14).

The message here is that noncontextual hidden variables cannot reproduce quantum theory's predictions. The predicted violations have also been tested in experiments, and the results are consistent with quantum theory's predictions.[27]

[27] Examples include Ahrens *et al* (2013) and Lapkiewicz *et al* (2011).

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