A Kochen-Specker inequality from a SIC

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Yu and Oh [1] have given a state-independent proof of the Kochen-Specker theorem in three dimensions using only 13 rays. The proof consists of showing that a non-contextual hidden variable theory necessarily leads to an inequality that is violated by quantum mechanics. We give a similar proof making use of 21 rays that constitute a SIC and four Mutually Unbiased Bases.

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Introduction.—The Kochen-Specker theorem states that a certain kind of hidden variable theory cannot be consistent with quantum mechanics. The idea is to assign truth values (1 for true, 0 for false) to a finite set of measurements represented by projectors onto rays in Hilbert space. These assignments must obey the Kochen-Specker rules, namely no two orthogonal projectors can both be true, and one member of each complete orthonormal basis must be true. Since two orthogonal projectors commute they represent compatible measurements. Note that the assignment made for a particular projector is independent of which particular set of mutually compatible measurements it belongs to—even though it may belong to several such contexts. Such a hidden variable theory is said to be non-contextual.

The usual proof proceeds by finding a finite set of projectors with a pattern of orthogonalities such that there does not exist a truth value assignment consistent with quantum mechanics. The idea is to use the rules [2, 3]. In other words, a non-contextual hidden variable theory reproducing the quantum mechanical results is shown to be logically impossible. The smallest number of projectors needed for such a proof seems to be 18 (in four dimensions [4]), or 31 (in three dimensions [5]).

Klyachko et al. [6] noticed that, using only five projectors in three dimensions, the Kochen-Specker rules lead to an inequality for observed frequencies that can be violated in quantum mechanics, if a particular quantum state is chosen. It was further observed that one can find a set of projectors so that, without employing the Kochen-Specker rules, they lead to an inequality violated by all quantum states (including the totally mixed state) [7]. In fact any version of the usual proof leads to such an inequality [8]. We call the first type of inequality a Kochen-Specker inequality and the second type, where the truth value assignments are constrained only by the assumption of non-contextuality, a non-contextual inequality. Yu and Oh [1] found a state-independent Kochen-Specker inequality from 4 projectors chosen from a larger set of 13, and a state-independent non-contextual inequality from the same set.

It is difficult to prove experimentally that something is logically impossible. On the other hand the reformulation of the Kochen-Specker theorem in terms of inequalities has led to a number of recent experimental tests [9–13]. Using inequalities also has the incidental advantage that the Kochen-Specker theorem can be proved over the rational numbers [14].

Our purpose is to give a state-independent proof along the same lines as Yu and Oh, but starting from a configuration of rays in three dimensions that is of independent interest: a symmetric informationally-complete POVM (SIC) and a complete set of mutually unbiased bases (MUB). The resulting configuration of 21 rays is highly symmetric, and we believe that it has some advantages.

Our 21 vectors.—Let \( q = e^{2\pi i/3} \), a third root of unity. In unnormalised form the first nine vectors are

\[
(0, 1, -1) \quad (0, 1, -q) \quad (0, 1, -q^2)
\]

\[
(-1, 0, 1) \quad (-q, 0, 1) \quad (-q^2, 0, 1)
\]

\[
(1, -1, 0) \quad (1, -q, 0) \quad (1, -q^2, 0)
\]

These vectors form a POVM, a set of vectors such that if one sums all the projectors \(|\psi_i\rangle\langle\psi_i|\) one obtains an operator proportional to the unit matrix. In fact they form a SIC [15, 16]. For our purposes, a SIC in dimension \( N \) is simply a collection of \( N^2 \) unit vectors such that

\[
\sum_{i=1}^{N^2} |\psi_i\rangle\langle\psi_i| = N \mathbb{1}
\]

(2)

\[
|\langle\psi_i|\psi_j\rangle|^2 = \frac{1}{N+1} \quad \text{if} \quad i \neq j
\]

(3)

A SIC is a very special kind of POVM. There is much more to say about the two notions we just introduced—they are used to describe measurements of a more general kind than the usual von Neumann measurements—but in
this letter none of this is relevant. The measurements we are thinking of are ordinary projective measurements.

We use twelve further vectors that can be collected into four bases. Again in unnormalized form they are the columns of the matrices

\[
\Delta^{(0)} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \Delta^{(\infty)} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & q & q^2 \\ 1 & q^2 & q \end{bmatrix},
\]

\[
\Delta^{(1)} = \begin{bmatrix} 1 & q^2 & q \\ q^2 & 1 & q^2 \\ q^2 & q^2 & 1 \end{bmatrix}, \quad \Delta^{(2)} = \begin{bmatrix} 1 & q & q \\ q & 1 & q \\ q & q & 1 \end{bmatrix}.
\]

These four bases have a particular relation to each other, and form a complete set of MUB \[17, 18\]. Again this is irrelevant here.

What is relevant is the special relationship that the SIC and the MUB enjoy in three dimensions. As was noted some time ago [19], each of the twelve MUB vectors is orthogonal to three SIC vectors in such a way that each basis divides the SIC vectors into three distinct sets. Moreover each SIC vector is orthogonal to four MUB vectors, one from each basis. This pattern of orthogonalities is sometimes referred to as the Hesse configuration; we will comment on this later.

A state-independent Kochen-Specker inequality.—Our first inequality will concern the SIC vectors only, but we constrain their truth values by first assigning truth values to the basis vectors. The Kochen-Specker rules force us to distribute one “1” and two “0s” among the three vectors in each of the four bases. Because each such vector is orthogonal to three SIC vectors this will force us to assign “0” to some of the latter.

Let us see how this works. We think of the SIC vectors as nine points in a square array arranged as in (1). In the figures the lines represent basis vectors. The three SIC vectors orthogonal to a given basis vector lie on the corresponding line. A solid line represents a basis vector assigned “1”, and the orthogonalities then force the SIC vectors on that line to be assigned “0” (as shown by filled dots). In Fig. 1 we do this first for \( \Delta^{(0)} \) and then for \( \Delta^{(\infty)} \). SIC vectors whose assignments are still undetermined are shown as empty dots.

\begin{修养}
\begin{figure}
\includegraphics[width=\textwidth]{figure1.png}
\caption{Truth value assignments from \( \Delta^{(0)} \) and \( \Delta^{(\infty)} \).}
\end{figure}
\end{修养}

For readers familiar with the Kochen-Specker literature, we emphasise that these are not orthogonality graphs [2].

We had a choice when we assigned truth values to the MUB vectors, but by the symmetry of the problem the choices made for the first two bases did not matter. When we proceed to \( \Delta^{(1)} \) and \( \Delta^{(2)} \) the choices do matter, but there are only nine possible choices and one quickly goes through them all. One possibility is shown in Fig. 2. Some of the “lines” now look curved; for readers familiar with such things we remark that they are in fact lines in a finite affine plane [18].

\begin{修养}
\begin{figure}
\includegraphics[width=\textwidth]{figure2.png}
\caption{Truth value assignments from \( \Delta^{(1)} \) and \( \Delta^{(2)} \).}
\end{figure}
\end{修养}

In this case seven SIC vectors are assigned the value “0”, and two SIC vectors are left undetermined. This will happen for eight out of the nine choices. In the remaining case all SIC vectors are assigned “0”.

Using a single projective measurement we can determine the truth value of at most one SIC vector. Let \( T_i \) be the truth value of the SIC vector \(|\psi_i\rangle\). When we repeat the experiment many times we divide the ensemble into nine subensembles. Assuming that this does not affect the averages, we conclude that their sum cannot exceed 2. Thus

\[
\sum_{i=1}^{9} \langle T_i \rangle \leq 2 .
\]

This is the prediction from any non-contextual hidden variable theory. But the quantum mechanical average, if the state of the system is \( \rho \), is

\[
\sum_{i=1}^{9} \text{tr} \rho |\psi_i\rangle \langle \psi_i| = \text{tr} \rho \sum_{i=1}^{9} |\psi_i\rangle \langle \psi_i| = 3 ,
\]

by eq. (2). Should experiments confirm this, the hidden variable theories have been falsified.

A state-independent non-contextual inequality.—It is possible to write down an inequality that does not assume the Kochen-Specker rules, and which is violated by quantum mechanics. The only assumption made in deriving such a non-contextual inequality is that the hidden variable theories assign values to 21 dichotomic observables in a non-contextual manner.

We choose to represent the 21 quantum mechanical observables by the 21 operators

\[
\begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{bmatrix}, \quad
\begin{bmatrix}
1 & 1 & 1 \\
1 & q & q^2 \\
1 & q^2 & q
\end{bmatrix},
\]

\[
\begin{bmatrix}
1 & q^2 & q \\
q^2 & 1 & q^2 \\
q^2 & q^2 & 1
\end{bmatrix}, \quad
\begin{bmatrix}
1 & q & q \\
q & 1 & q \\
q & q & 1
\end{bmatrix}.
\]
\[ A_i = 1 - 2|\psi_i\rangle\langle\psi_i| , \] (7)

with the spectrum \((1, 1, -1)\). We also introduce the dichotomic hidden variables \(a_i\), taking the values \(\pm 1\).

Let us introduce the symbol \(\Gamma_{ij}, 1 \leq i, j \leq 21\), which by definition is equal to 1 if the measurements labelled \(i\) and \(j\) are compatible and distinct (that is if \(A_i\) and \(A_j\) commute), and equal to 0 otherwise. We are interested in the function

\[ C = \sum_{i=1}^{21} a_i - \frac{1}{5} \sum_{i,j=1}^{21} \Gamma_{ij} a_i a_j . \] (8)

There are \(2^{21}\) different assignments one can make for the \(a_i\)’s, but since our configuration is very symmetric an exhaustive search is not difficult. The conclusion is that \(C\) takes values no larger than \(\frac{63}{5}\). Hence when we take averages, the hidden variable theory predicts that

\[ \sum_i \langle A_i \rangle - \frac{1}{5} \sum_{i,j} \Gamma_{ij} \langle A_i A_j \rangle \leq \frac{63}{5} . \] (9)

In quantum mechanics this quantity is evaluated as the expectation value of the operator

\[ Q = \sum_i A_i - \frac{1}{5} \sum_{i,j} \Gamma_{ij} A_i A_j = \frac{67}{5} \mathbb{1} . \] (10)

A minor calculation is needed to show this. Hence the quantum expectation value is again independent of the state, and given by

\[ \sum_i \text{tr} \rho A_i - \frac{1}{5} \sum_{i,j} \Gamma_{ij} \text{tr} \rho A_i A_j = \text{tr} \rho Q = \frac{67}{5} . \] (11)

This is an obvious violation of the prediction from the non-contextual hidden variable theories, which is that this average should be less than or equal to \(\frac{43}{5}\).

Comments.—We end with four comments.

a) The inequality we have presented is not unique. We could have considered the quantity

\[ C = \sum_i a_i - k \sum_{i,j} \Gamma_{ij} a_i a_j , \quad \frac{1}{8} < k < \frac{1}{4} , \] (12)

and we would still have obtained a violation. We can also weight the individual terms differently. Such considerations are important if one wants an experimentally robust inequality to test.

b) The 13 vectors appearing in the proof by Yu and Oh \[1\] are real. They include the computational basis, two triplets of vectors that can be extended to complete SICs in complex Hilbert space, and a set of four vectors that are unbiased with respect to the computational basis. The latter four form a POVM, and play the role that the SIC vectors play in our construction.

c) The Hesse configuration is normally not thought of as a pattern of orthogonalities, but as a collection of nine vectors and twelve two-dimensional subspaces (normal to the MUB vectors), such that each subspace contains three vectors and each vector belongs to four subspaces. It is interesting to observe that a somewhat similar configuration of vectors and subspaces, known as the Reves configuration, is relevant \[20\] to Peres’ 24-ray proof \[3\] of the Kochen-Specker theorem in four dimensions.

d) The close connection between SICs and mutually unbiased bases that we have used appears to be special to three dimensions \[21 \, 22\]. At the same time we note that there is a foundational aspect to SICs \[23\]. We do not know if our observation can be employed in that context.

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