Gleason, Kochen-Specker, and a competition that never was

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Abstract. I review the two theorems referred to in the title, and then suggest that it would be interesting to know how much of Hilbert space one can use without forcing the proof of these theorems. It would also be interesting to know what parts of Hilbert space that are essential for the proofs. I go on to discuss cubes, graphs, and pentagrams.

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GLEASON

Gleason’s theorem [1] is one of the key structural theorems of physics. Gleason assumes that the projective Hilbert space description of quantum states is in place, and then proves that there exists exactly one way to introduce probabilities in this description, namely the usual way through a density matrix. More precisely each orthonormal basis is associated to a probability distribution which then governs projective measurements (so that we will tend to use the expressions “orthonormal basis” and “projective measurement” a little interchangeably). Here is one possible formulation of the theorem:

Gleason’s theorem. In a real or complex Hilbert space of dimension \( N > 2 \), let each ray \( |\psi\rangle \langle \psi| \) be assigned a real number \( p_\psi \geq 0 \), such that

\[
\sum_{i=1}^{N} p_{e_i} (|e_i\rangle \langle e_i|) = 1
\]

whenever the vectors \( \{ |e_i\rangle \}_{i=1}^{N} \) form an orthonormal basis. Then there exists a density matrix \( \rho \) such that

\[
p_\psi = \text{Tr} \rho |\psi\rangle \langle \psi|
\]

for all unit vectors \( |\psi\rangle \).

A ray is a one-dimensional subspace, spanned by a single vector and represented by a projector. The real valued function \( p_\psi \) is called a frame function. There are no further assumptions, in particular continuity is proved, not assumed. For this reason the proof of Gleason’s theorem is famously difficult. At the same time it should be stressed that from the point of view of physics the assumptions are quite strong. It is assumed that the number \( p_\psi \) remains the same regardless of which, out of many, orthonormal bases it is regarded as being part of. The technical term for this is that the probabilities are “non-contextual”. Perhaps—as stressed by Bell [2, 3]—this need not be the case? In any case the theorem highlights how much one can get out of this assumption.

The theorem dates from 1957. It is worth noticing that had it been a little weaker, so that we were left with a one parameter family of ways in which probability distributions could be extracted from the formalism, then we would have seen a very large number of experiments trying to set bounds on that parameter. The theorem has figured prominently in the literature on the foundations of quantum mechanics [4], and it is possible to dig deeper [5], but my purpose here is a little orthogonal to what has gone on before.

KOCHEN-SPECKER

Gleason’s theorem has a corollary with an independent proof [6, 7]:

The Kochen–Specker theorem. It is impossible to assign all rays of an \( N > 2 \) dimensional Hilbert space a truth value (true or false), in such a way that exactly one vector in each orthonormal basis is true.
The second theorem is a corollary of the first, because if we replace true and false by one and zero, we have an example of a frame function that obeys Gleason’s conditions. But probability distributions that come from density matrices are not of this form. It is a very interesting corollary, since the outcome of a projective measurement does provide such truth value assignments to the vectors in the given orthonormal basis. Apparently then these assignments did not exist prior to the decision to perform that particular measurement. To the extent that one can talk about them all, they are necessarily contextual even though the probabilities are not.

Ernst Specker’s original motivation concerned a problem in theology: can God know the outcome of all events, also those that could have happened but in fact did not? The answer from quantum mechanics is a clear no. This is usually stated somewhat lesscosmically as a colouring problem. By convention red corresponds to true, and green corresponds to false. The theorem then says that it is impossible to colour the rays of Hilbert space using two colours only consistently with the rule derived from eq. (1), namely that exactly one vector in each orthonormal basis must be coloured red.

The proof is famously easy, and proceeds by exhibiting a finite number of uncolourable vectors, including some orthonormal bases. In their original proof Kochen and Specker used a set of 117 rays for this purpose. Naturally this led to a competition: who can prove the Kochen-Specker theorem with the smallest number of rays? The upshot in dimension 3 was that Schütte [8], Peres [8], and Penrose [9] produced uncolourable sets with 33 rays, while Conway and Kochen produced one with 31 rays [8]. In four dimensions Peres produced an elegant set with 24 [10], Kernaghan one with 20 [11], and Cabello et al [12] a set with 18 rays. Exhaustive computer searches [13] have since confirmed that Cabello et al are the winners.

Several of these finite sets form seducingly beautiful configurations. While this is incidental to our understanding of quantum mechanics, it does add to the charm of the subject. We will go into the details of the Peres and Penrose sets later. It is perhaps worth mentioning that Peres’ set of 24 rays form two triplets of mutually unbiased bases. Other sets involving such bases have been produced subsequently, systematically in four [14] and also in eight [3, 15] dimensions. The vectors involved in these constructions are eigenvectors of operators belonging to a Weyl-Heisenberg group, and in dimensions not equal to a power of a prime number things work out differently [16]—although in dimension three the Weyl-Heisenberg group does have something special to offer [17].

**THE COMPETITION THAT NEVER WAS**

Given that it is impossible to colour all of Hilbert space according to the Kochen-Specker rules we ask: how much of it can be coloured? As rules, we choose to require that no two orthogonal vectors are red, and no orthonormal basis has all its vectors green, but it is allowed to leave some vectors uncoloured. Moreover it is understood that the red and green regions should be measurable, and the uncoloured region (that must perforce exist) should be measurable too.

As far as I know only one paper, by Appleby [18], has been devoted to this question. It confined itself to three dimensional real Hilbert space, so colouring the unit vectors is equivalent to colouring a 2-sphere (or more precisely a real projective 2-space). One of its purposes was to provide a lower bound for the area that must be left uncoloured. By wiggling one of the uncolourable configurations employed to prove the Kochen-Specker theorem a lower bound of around one percent was achieved. It was also noted that 87 percent of the sphere can be coloured consistently with the rules. The idea is to start with a vector and colour it red, and then colour all vectors orthogonal to it green. Pictorially the North Pole is red and the equator is green. Then one enlarges the North Pole to a red polar cap, keeping it small enough so that one cannot place two orthogonal vectors there, and at the same time one creates a green belt around the equator, keeping it small enough so that it remains impossible to place a complete orthonormal set of vectors there. The polar cap then extends down to a latitude of 45 degrees, and the belt goes up to a latitude of 35 degrees. The sum of the area of the cap and the belt turns out to be 87 % of the total area of the sphere.

This idea can be extended to real Hilbert spaces of arbitrary dimension [19]. Interestingly the end result is not at all obvious, since it depends on a delicate balance between two opposing effects: the width of the green belt shrinks as the dimension grows, but at the same time the volume of the sphere becomes concentrated to a region around the equator. As a result the fraction of the sphere that can be coloured in this way shrinks down to 67 % (for dimension 12), and then raises slowly to its limiting value

\[ \mu_\infty = \text{erf} \left( \frac{1}{\sqrt{2}} \right) \approx 0.68 . \]  

(3)
A similar strategy can be followed for complex Hilbert spaces of arbitrary dimension $N$. We write a unit vector modulo phases as

$$
\psi = (\sqrt{p_0}, \sqrt{p_1}e^{i\nu_1}, \ldots, \sqrt{p_{N-1}}e^{i\nu_{N-1}})^T, \quad \sum_{i=0}^{N-1} p_i = 1.
$$

These coordinates are very convenient for volume calculations using the Fubini-Study measure, since they make projective Hilbert space behave like a product of a flat simplex and a flat torus of a standard size. We can now make a red polar cap including

$$
1 \geq p_0 > \frac{1}{2}.
$$

We can also make a green belt extending between

$$
0 \leq p_0 < \frac{1}{N}.
$$

Using the Fubini-Study measure to compute volumes one finds that this colouring covers a fraction of projective Hilbert space which is

$$
\mu_N = 1 - \left(1 - \frac{1}{N}\right)^{N-1} + \left(\frac{1}{2}\right)^{N-1}.
$$

For $N = 3$ this is 81%, slightly less than in the real case. It reaches a minimum of 61% for $N = 9$, and then raises slowly towards the limit

$$
\lim_{N \to \infty} \mu_N = 1 - \lim_{N \to \infty} \left(1 - \frac{1}{N}\right)^{N-1} = 1 - \frac{1}{e} \approx 0.63.
$$

This result was never published since at this point its author decided she did not want to be a physicist, she wanted to be a poet. To those who can read Swedish I can recommend Osäkerhetsrelationen, a book-length poem on the foundations of quantum mechanics [20].

But as a result no attempt to beat Appleby’s construction, and to colour more of Hilbert space than he did, has been made. I think people ought to compete with him. A list of attempts to do better than him might well provide interesting food for thought, in many ways even more interesting than the list of examples of finite sets of uncolourable vectors. Actually my suspicion is that Appleby’s construction may well be optimal at least in high dimensions, but nevertheless such a competition might shed light on the next question.

Of course one can adopt other rules of the game if one wants to. In particular, Granström asked what fraction of all orthonormal bases that can be fully coloured according to the Kochen-Specker rules. Using Appleby’s colouring she found that percentage to be 69% in the real three dimensional case, and 34% in the real four dimensional case [19]. Possibly this fraction does go to zero as the dimension increases?

**WHAT CAN YOU COLOUR?**

It is striking that most of the known finite sets of uncolourable vectors, in particular all the ones with close to the minimal number of entries except the Penrose set, contain real vectors only. In four dimensions there is a definite meaning attached to this: it is known that given a set of real vectors one can find a tensor product decomposition such that all of them are maximally entangled, and conversely given a maximally entangled set of vectors it is possible to choose a magical basis such that they become real [21]. There is a similar interpretation of real vectors in three dimensions: they are maximally non-coherent with respect to a definite definition of spin coherent states [22]. So we already know that the set of all maximally entangled states is uncolourable.

The set of separable two-qubit states is colourable however. To see this, note that any separable state $|\psi_A\rangle \otimes |\psi_B\rangle$ can be coordinatized by

$$
|\psi_A\rangle = \cos \frac{\theta_A}{2} |0\rangle + \sin \frac{\theta_A}{2} e^{i\phi_A} |1\rangle,
$$

$$
(9)
$$
and similarly for $|\psi_B\rangle$. Now divide the set of separable states into four sets,

$$
I : (\phi_A, \phi_B) \in [0, \pi) \times [0, \pi) , \quad II : (\phi_A, \phi_B) \in [0, \pi) \times [\pi, 2\pi) ,
$$

$$
III : (\phi_A, \phi_B) \in [\pi, 2\pi) \times [0, \pi) , \quad IV : (\phi_A, \phi_B) \in [\pi, 2\pi) \times [\pi, 2\pi) .
$$

There are no orthogonalities within these sets, so we can colour the first set red and the other sets blue.

This suggests an alternative strategy for colouring a four dimensional Hilbert space, namely to start by colouring the separable states and then to work outwards from there. Will this beat Appleby’s strategy? Will it lead to a larger fraction of coloured bases?

**A COMMENT ON IMPOSSIBLE CUBES**

The Penrose set of 33 vectors is special in that it cannot be made real by any choice of basis. This goes a little against the drift of the idea that it should be the real vectors that resist colouring the most, but on closer inspection one finds that this set is complex only in a mild way. Let us recall how the Penrose set, and that of Peres, arises. In his print *The Waterfall*, M. C. Esher illustrates one of the Penrose’s impossible pictures [23]. Of concern for the moment are the three interlocking cubes that grace the top of one of the towers in Escher’s print. We observe that a cube is naturally associated to $3 + 6 + 4 = 13$ rays, three going through the middle of a face, six through the middle of an edge, and four connecting the corners. This gives rise to an interesting orthogonality graph with 13 vertices representing the rays. In such a graph each vertex represents a vector, and the vertices are connected with a link if and only if they represent orthogonal vectors. (The converse problem, to find the lowest dimension in which a given graph can be realized as an orthogonality graph, is non-trivial.) The Kochen-Specker rules ask us to colour the vertices of such a graph red or green, subject to the rules that two linked vertices cannot both be red, and any complete triangle must contain exactly one red vertex (if we are in three dimensions, where three mutually orthogonal vectors form a basis). The cube graph is colourable—but still very interesting in that it leads to a state-independent probabilistic proof of the Kochen-Specker theorem. This was discovered recently by Yu and Oh [24], and discussed in Larsson’s talk, but I will not go into this now. I just observe that in this connection the graph is a way to visualize the cube, and I also observe that the vectors are determined uniquely up to an overall unitary transformation by the orthogonalities encoded in the graph.

The impossible cubes that appear in Escher’s print arise if you start with one cube, and add two cubes obtained by rotating the first cube ninety degrees around an axis that connects two opposing edges. A pair of two orthogonal axes of this kind is needed to produce the three interlocking cubes. Each new cube gives rise to ten new vectors, while three vectors are shared by all three cubes, so the total number of vectors appearing in the print equals 33. Six intercube orthogonalities arise, and this turns out to be just enough to make the completed orthogonality graph uncolourable.

**FIGURE 1.** The Escher-Peres interlocking cubes. Each 13-vertex triangle is a copy of the Yu and Oh graph, including 24 orthogonalities given by the links. Reproduced with permission [25].

In the basis provided by the three vectors common to all three cubes the second cube is obtained from the first by
\[
R_{I \rightarrow II} = \begin{pmatrix}
e^{i\phi} & 0 & 0 \\
0 & 0 & -1 \\
0 & 1 & 0
\end{pmatrix}
\] (11)

and the third from the first by

\[
R_{I \rightarrow III} = \begin{pmatrix}
0 & 0 & -1 \\
0 & e^{-i\phi} & 0 \\
1 & 0 & 0
\end{pmatrix}
\] (12)

—and we took the liberty to add an undetermined phase factor, since this leaves all the orthogonality relations in place. The complex Penrose set can now be obtained from the Peres set by a suitable choice of this free phase [26]. It seems right to say that the former is only mildly complex. Incidentally the fact that there is a free phase in the realization of the orthogonality graph seems to be unusual, given that the graph is sufficiently involved to give a proof of the Kochen-Specker theorem [27].

The remainder of Escher’s print illustrates a different holistic mathematical concept and is of no concern here, but it is clearly very appropriate for his print to include a proof of the Kochen-Specker theorem.

**Motivation**

After this pleasant excursion into the world of Art, let us return to Science. Does this circle of ideas have experimental consequences? In fact it has. To see this let us focus on a simple subgraph of the orthogonality graphs that we have encountered, namely the pentagon (or equivalently the pentagram). This is in fact a very interesting graph in itself, as was noted by Wright [28] and Klyachko et al. [29]. Moreover it occurs as a subgraph in the description of several “paradoxical” quantum arguments that have attracted the attention of experimentalists, including Hardy’s paradox [30] and the CHSH inequality [31, 32]. It is certainly colourable, but it should be observed that at most two vertices can be coloured red, meaning that at most two of the potential outcomes can come out as “true”.

Now consider a classical experiment, with measurements \( P_i \) whose outcomes obey the Kochen-Specker rules. We can imagine a platter with a pentagram drawn on it, and five cups placed upside down over the vertices. Each time the platter is presented to us we look under two cups connected by a link, and record the number of stones (1 or 0) found under each cup. It never happens that there are stones under both cups, and from this fact—assuming that our choice of which pair of cups we look under has nothing to do with the preparation of the platter—we reason that the total number of stones on the platter never exceeds 2. After many trials we then expect

\[
\sum_{i=1}^{5} \langle P_i \rangle \leq 2.
\] (13)

But in a corresponding quantum experiment the measurements correspond to projectors \( \hat{P}_i \) with orthogonality properties given by the graph. The latter restrict the spectrum of the operator

\[
\Sigma = \sum_{i=1}^{5} \hat{P}_i
\] (14)
in such a way that the maximal eigenvalue of \( \Sigma \) never exceeds \( \sqrt{5} \) [22, 30]. We therefore find the quantum bound

\[
\sum_{i=1}^{5} \langle \psi | \hat{P}_i | \psi \rangle = \langle \psi | \Sigma | \psi \rangle \leq \sqrt{5}.
\] (15)

We can exceed this bound with the classical platter if it is prepared in a conspiratorial way: only one stone is used in the preparation, but it is always placed under one of the two cups we will decide to look under. Thus we get

\[
\text{classical bound} = 2 < \text{quantum bound} = \sqrt{5} < \text{conspiratorial bound} = 2.5.
\] (16)

The Yu and Oh set of vectors (associated to the cube described earlier) lead to a similar inequality, but—like some other sets introduced earlier [33]—with the interesting difference that the projectors form an equal weights POVM, so that the classical bound is violated equally by all quantum states.
These bounds are testable. In fact they have been tested, and we will come back to this. In principle quantum mechanics is doubly on the line in such an experiment: the classical inequality could hold, or the quantum bound could be exceeded.

For systems whose Hilbert space dimension does not exceed four so many transformations have been done in the lab that it is completely unreasonable to expect any problems with the quantum mechanical description. However, from some points of view higher dimensional Hilbert spaces are very mysterious. In particular they are that from a point of view that I myself often adopt, that of Mutually Unbiased Bases (MUBs) and Symmetric Informationally Complete POVMs (SICs). There does exist a research program aiming to reconstruct Hilbert space from SICs [34], but it is conceivable that SICs do not exist in dimension 77 (say). Does this mean that such research programs run the risk of reconstructing something that is only approximately a Hilbert space, and if so what do we do? Is it obvious that we will stick to Hilbert space? For MUBs these questions arise already in dimension 6.

Some of the pioneers in testing the Bell inequalities did expect them to hold, and quantum mechanics to fail [35]. Nobody expects this to happen in a pentagram experiment, but I am suggesting that we have as yet no reason to be dogmatic about the outcome of similar experiments for higher dimensional systems.

**REMARKS ON GRAPHS**

So far I have not even hinted whether the construction of “paradoxical” graphs is an art or a science. Actually it turned into a science quite recently, and it by now known what properties a graph must have in order to give rise to Kochen-Specker inequalities of the kind I have discussed. In particular, what we have called the classical, the quantum, and the conspiratorial bounds turn out to be identical with quantities that have been studied by graph theorists [31]. They are known respectively as the independence number (defined as the maximum number of pairwise disconnected vertices in the graph), the Lovász theta-function [36], and the fractional packing number. The Lovász theta-function can be obtained by semi-definite programming, so the quantum bound can be effectively computed. This is interesting because the problem of finding the classical bound—while easy enough for small graphs—turns out to be NP complete. This cross-disciplinary discovery have made some powerful tools available to the quantum theorist, and many developments stem from here. It would take us too far afield to try to account for them here.

One important point, that I should mention, is that many recent experiments are aiming not at the inequality (13) (and its relatives for other graphs) but at correlation inequalities that can be derived without reference to the Kochen-Specker rules. They depend only on the assumption of pre-determined outcomes [29], but again I will not go into this here.

**EXPERIMENTS**

So far two quantum optical experiments have been made to test the pentagram inequality [37, 38]. As soon as one looks at such an experiment in the lab, one begins to appreciate the force of the comment that “the result of an experiment may reasonably depend not only on the state of the system ... but also on the complete disposition of the apparatus”. This quote is not from Bohr, it is Bell [2] questioning the assumption that a hidden variables theory must be non-contextual, or whether the outcome of the measurement associated to \( P_2 \) might depend on which of the mutually incompatible measurements \( P_1 \) and \( P_3 \) it is measured together with (given that it is compatible with both).

Both experiments prepare a state that should lead to a maximal violation of the classical bound, and the results are in quite good agreement with what one would expect. Still, though beautiful, the experiments do fall short of the ideal. They perform compatible measurements—say ten thousand measurements—in pairs, beginning with \( P_1 \) and \( P_2 \), going on to \( P_2 \) and \( P_3 \), and so on, ending with \( P_3 \) and \( P_1 \). It would be desirable to let a random generator decide each time what pair of measurements that is to be performed, in order to stymie any conspiratorial preparation of the classical platter. In the first experiments there is also the difficulty that the measurement performed together with \( P_3 \) is not in fact identical to the measurement \( P_1 \), and special measures must be taken to deal with this. In effect one of the vertices of the pentagram does not close. You may recall that it was precisely through such an open vertex that the devil got into Faust’s pentagram [39].

There is room for further refinements of these experiments. I expect that many years will pass before we can listen to a talk entitled “towards a loop-hole free contextuality test”. Still the refinements are important, and will serve as preparation for the day when such an experiment can be done for six dimensional systems—where quantum mechanics just possibly may begin to crack.
FIGURE 2. An experimental afterthought. With apologies to George Gamow, and to the organizers of the Pauli session.

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