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PENTAGRAMS AND PARADOXES

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Abstract

Klyachko and coworkers consider an orthogonality graph in the form of a pentagram, and in this way derive a Kochen-Specker inequality for spin 1 systems. In some low-dimensional situations Hilbert spaces are naturally organised, by a magical choice of basis, into $SO(N)$ orbits. Combining these ideas some very elegant results emerge. We give a careful discussion of the pentagram operator, and then show how the pentagram underlies a number of other quantum "paradoxes", such as that of Hardy.

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1. Introduction

We will be interested in five unit vectors. Counting them modulo 5 we assume the orthogonality relations

$$\langle k|k+2\rangle = 0 \ , \qquad k \in \{0, 1, 2, 3, 4\} \ . \tag{1}$$

To visualise this we draw an orthogonality graph, where each node represents a vector and each link an ortogonality relation. Our orthogonality graph is therefore a pentagram—or a pentagon, depending on how we draw it (see Fig. 1). The pentagram operator is

$$\Sigma \equiv \sum_{i=0}^{4} |k\rangle\langle k| \ . \tag{2}$$

The dimension of Hilbert space is assumed to be 3 or 4, so that the pentagram vectors form an overcomplete set, and in fact a frame of a peculiar kind.

In 3 dimensions any pair of vectors uniquely determines a third ray, a vector up to phase. In this way a non-degenerate pentagram uniquely determines 5 orthogonal triads. These were used by Wright in an interesting contribution to quantum logic [1, 2]. He explored probability assignments consistent with Gleason's rules, and found that for the pentagram there exists assignments that are inconsistent with quantum mechanics when the graph is embedded in a full Hilbert space.

This is already enough to show that something interesting can be done with pentagrams. More recently Klyachko and coworkers [3, 4] derived a pentagram inequality that—following Kochen and Specker [5]—shows quantum mechanics to be probabilistically inconsistent with an underlying non-contextual reality. Here is their argument in a slightly modified form [6]: The Kochen-Specker rules demand that each node in the graph is assigned a value 0 or 1 (a preassigned truth value), in such a way that orthogonal vectors are never both assigned the value 1, and such that the sum of the values in any orthogonal basis equals 1. When the same assignments are carried over to the projectors in the pentagram operator we see that at most two of them can be assigned the value 1. In a non-contextual reality an experimenter, when adding observed frequencies of the five projectors she can measure, will therefore always find that

$$\langle \Sigma \rangle \leq 2 \ , \tag{3}$$

regardless of how she prepares her state. The point of course is that the quantum expectation values of Σ will violate this bound for appropriately chosen states.

In section 2 we give a thorough discussion of the three dimensional pentagram operator. In section 3 we impose additional restrictions on the frame vectors. Thus we can insist that they all share the same degree of entanglement, or spin coherence. If we use the magical basis, available in 3 and 4 dimensions, maximally entangled or non-coherent states are real vectors, and conversely [7, 8, 4]. We can always form a pentagram from real vectors. In 3 dimensions we then find the beautiful feature that every non-coherent state will violate some pentagram inequality [4]—in complete analogy with the fact that every entangled state in four dimensions violates some Bell inequality. In sections 4 and 5 we go on to show that the pentagram inequality unifies several quantum "paradoxes" with slightly more involved orthogonality graphs. This includes a graph used by Kochen and Specker themselves [10], the Aharon-Vaidman game [11], and Hardy's paradox [12]. In section 6 we briefly discuss the four dimensional pentagram operator, and finally suggest some open questions that we find interesting.
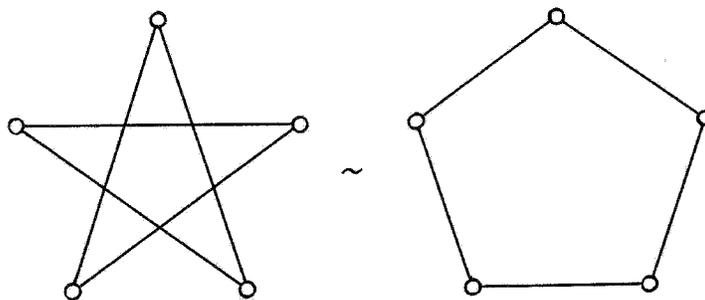

Figure 1: Two equivalent ways to draw our orthogonality graph. Since orthogonal vectors are far apart the pentagram is arguably a more "realistic" picture.

2. The pentagram operator

The largest violation of the KS inequality (3) will always be achieved by the eigenvector corresponding to the largest eigenvalue, so with a view to understand what violations are possible we first discuss the possible spectra of the pentagram operator Σ. A quick way to see what spectra can occur is the following. Define

$$p_{k,k+1} = |\langle k|k+1 \rangle|^2 \ . \tag{4}$$

A calculation shows that

$$\mathrm{Tr}\Sigma = 5 \qquad \mathrm{Tr}\Sigma^2 = 5 + 2A \qquad \mathrm{Tr}\Sigma^3 = 5 + 6A \ , \tag{5}$$

where

$$A = \sum_{k=0}^{4} p_{k,k+1} \ . \tag{6}$$

Assuming that the dimension of Hilbert space is three, the eigenvalues of Σ therefore obey the characteristic equation

$$P_3(\lambda) = \lambda^3 - 5\lambda^2 + (10 - A)\lambda + 3A - 10 = 0 \ . \tag{7}$$

From this we see that there is a one parameter family of possible spectra labelled by the quantity A. So we need to know all possible values of A.

Let us therefore write down the most general set of five unit vectors obeying (1), and then compute A from the corresponding pentagram operator. We adapt a basis to the orthogonal vectors $|0\rangle$ and $|3\rangle$. Up to irrelevant phase factors we find the five column vectors

$$
\begin{array}{ccccc}
1 & \cos a & 0 & 0 & e^{-i\mu}\sin a\cos b/\sqrt{1 - s_a^2 s_b^2} \\
0 & 0 & \cos b & 1 & e^{-i\nu}\cos a\sin b/\sqrt{1 - s_a^2 s_b^2} \\
0 & e^{i\mu}\sin a & e^{i\nu}\sin b & 0 & -\cos a\cos b/\sqrt{1 - s_a^2 s_b^2}
\end{array}
\tag{8}
$$

We see that the set of all pentagrams is labelled by four angular variables. We will distinguish the two parameter set of real pentagrams for which all the five vectors are real, the one parameter set of real symmetric pentagrams

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for which $a = b$, and the regular pentagram for which the five real vectors form a cone with a regular pentagram as its base [3]. The pentagram is said to be degenerate if two of its projectors coincide.

The spectrum of an arbitrary pentagram operator is determined by

$$A = 2 - \frac{\sin^2 a \sin^2 b \cos^2 a \cos^2 b}{1 - \sin^2 a \sin^2 b} \ . \tag{9}$$

Evidently any allowed value of A and hence any spectrum can be obtained from a real pentagram, and in fact from a real symmetric pentagram. It is straightforward to show that

$$A_{\min} \leq A \leq 2 \ . \tag{10}$$

The maximum is obtained by a degenerate pentagram. The minimum $A_{\min} \approx 1.91$ is attained by the regular pentagram

$$\sin^2 a = \sin^2 b = \Phi - 1 \quad \Rightarrow \quad A = A_{\min} = 2 - \frac{1}{\Phi^5} \ , \tag{11}$$

where Φ is the Golden Mean

$$\Phi = \frac{1}{\Phi - 1} \ , \qquad \Phi = \frac{1 + \sqrt{5}}{2} \approx 1.618 \ . \tag{12}$$

We recall that the Golden Mean arises as the ratio between the sides of a triangle inscribed in a regular pentagon, with angles 72°, 72°, and 36°. The smaller triangle one of whose sides is obtained by taking the bisectrix of one of the larger angles is similar to the original triangle; this is how the equation for the Golden Mean arises.

The possible eigenvalues can now be computed explicitly as a function of the single variable $s = \sin a$, viz.

$$\lambda_0 = 2 - s^2 \ , \qquad \lambda_\pm = \frac{3 + s^2}{2} \pm \frac{1}{2} \sqrt{\frac{1 + 3s^2 - 5s^4 + s^6}{1 + s^2}} \ . \tag{13}$$

This is perhaps not so illuminating, so in Fig. 2 we display this one parameter family of spectra in an eigenvalue simplex. The largest possible eigenvalue is

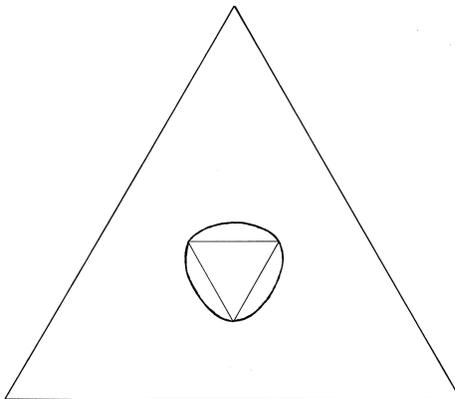$$\sqrt{5} \approx 2.236 \ . \tag{14}$$

Figure 2: The spectra of all possible pentagrams as a curve in the eigenvalue simplex. The sum of the eigenvalues equals 5. At a corner they would be $(5, 0, 0)$. The inscribed triangle has a corner at $(2, 2, 1)$ and contains spectra that would not violate the KS inequality, should they occur (they do not, except at the corners).

The corresponding pentagram is regular. Real vectors then violate the inequality provided their angle with the eigenvector giving maximal violation is less than $31°$; the pentagram vectors themselves give no violation.

The smallest possible eigenvalue is 1, and the spectrum $(2, 2, 1)$ results from degenerate pentagrams. These are the only ones that do not lead to any violation of the KS inequality (3). For later use we also observe that when $a = \epsilon$ is small the pentagram is almost degenerate and

$$\lambda_+ \approx 2 + \epsilon^2 \qquad \lambda_0 \approx 2 - \epsilon^2 . \tag{15}$$

These eigenvalues approach 2 at the same rate.

3. The magical basis

A vector in a complex Hilbert space can always be split into real and imaginary parts. Any vector can be written as

$$|\psi\rangle = \cos \sigma \mathbf{x} + i \sin \sigma \mathbf{y} . \tag{16}$$

But a physical state is represented by an equivalence class $|\psi\rangle \sim e^{i\phi}|\psi\rangle$ of unit vectors, and every equivalence class contains a representative such that

$$\mathbf{x}^2 = \mathbf{y}^2 = 1 \ , \qquad \mathbf{x} \cdot \mathbf{y} = 0 \ , \qquad 0 \le \sigma \le \frac{\pi}{4} \ . \tag{17}$$

The phase is thereby fixed up to a sign (unless $\sigma = \pi/4$). This works in all complex Hilbert spaces, but is usually of no interest because unitary transformations will not preserve the scalar product $\mathbf{x} \cdot \mathbf{y}$. But in 3 dimensions, if we are interested in spin coherent states, then we have restricted ourselves to the subgroup $SU(2) \sim SO(3)$ of the full unitary group. This is an experimentally motivated restriction in some circumstances [13]. Similarly, if we are interested in pairs of entangled qubits we are restricted to the local subgroup $SU(2) \times SU(2) \sim SO(4)$. In both cases a magical basis is, by definition, a basis in which $SO(N)$ is represented by real matrices [7]. Once a magical basis is adopted the parameter σ in eq. (16) is left unchanged by the transformations we do, and hence it labels the orbits of the relevant groups. We will refer to the quantity

$$C = |\langle \psi^\star | \psi \rangle| = \cos 2\sigma \tag{18}$$

as the concurrence of the state. The 'classical' orbit with $C = 0$ consists of spin coherent states in 3 dimensions, and of separable states in 4. Real vectors have $C = 1$ and are 'maximally non-classical'; in 4 dimensions these are the maximally entangled states.

There are various ways to substantiate the use of the adjective 'classical' here [4, 9]. A particularly relevant one, applicable in 3 dimensions, is the following [4]. First we restrict ourselves to pentagrams constructed from purely real vectors. The operator Σ is then real, and can be diagonalised by transformations belonging to the real rotation group $SO(3)$. They leave the concurrence, and the 'classicality' of the states, unchanged. For a general state (16) we tailor make a pentagram operator such that the eigenvector corresponding to the largest eigenvalue λ_1 is $\mathbf{x}$, and that corresponding to the second largest λ_2 is $\mathbf{y}$. Clearly

$$\langle \psi | \Sigma | \psi \rangle = \mathbf{x} \Sigma \mathbf{x} \cos^2 \sigma + \mathbf{y} \Sigma \mathbf{y} \sin^2 \sigma = \lambda_1 \cos^2 \sigma + \lambda_2 \sin^2 \sigma \ . \tag{19}$$

We now go back to Fig. 2 supplemented by eq. (15). Then we can convince ourselves that we obtain $\langle \Sigma \rangle = 2$ if and only if $\sigma = \pi/4$, that is for a coherent

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state, while all other states will violate its tailor made KS inequality. This is in complete analogy to the well known fact that all entangled states in 4 dimensions violate some Bell inequality [14].

4. Quantum paradoxes

If we begin to examine all the Kochen-Specker type arguments that have been put forward in the literature we see that pentagons are ubiquitous in the orthogonality graphs that underlie them. Thus, consider the graph in Fig. 3, which we refer to as the Kochen-Specker subgraph [5]. We assume that Hilbert space has 3 dimensions; then all the rays are uniquely defined once the five rays in the upper pentagon are given.
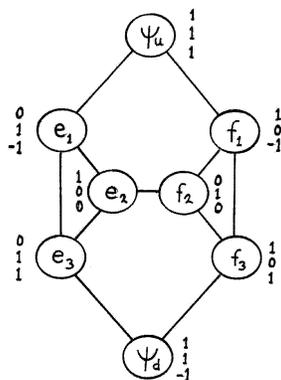

Figure 3: The Kochen-Specker subgraph. In 3 dimensions the upper pentagon completely determines the lower. An explicit realisation maximising the amount by which $|\psi_d\rangle$ violates the upper pentagram inequality is shown.

The Kochen-Specker rules make it impossible to assign the value 1 to both the upper and the lower vector. In a non-contextual reality the system cannot have the properties corresponding to these two projectors at the same time. Nevertheless it is a realisable graph. With the choice of vectors shown in the figure we obtain

$$p = |\langle\psi_u|\psi_d\rangle|^2 = \frac{1}{9} \; . \tag{20}$$

This is a probabilistic violation of non-contextual reality [15]. It is also the maximal violation that one can obtain from this graph. Our point here is that maximising p is equivalent to maximising the amount by which $|\psi_d\rangle$ violates the pentagram inequality for the upper pentagon in the graph. The proof is simple. As shown in Fig. the graph contains two ortogonal triads $|e_i\rangle_{i=1}^3$ and $|f_i\rangle_{i=1}^3$. Evidently

$$\langle\psi_d|e_1\rangle\langle e_1|\psi_d\rangle + \langle\psi_d|e_2\rangle\langle e_2|\psi_d\rangle = \langle\psi_d|\psi_d\rangle - \langle\psi_d|e_3\rangle\langle e_3|\psi_d\rangle = 1 \ , \qquad (21)$$

and similarly for the other triad. It follows that

$$\langle\psi_d|\Sigma_u|\psi_d\rangle = \langle\psi_d|\psi_u\rangle\langle\psi_u|\psi_d\rangle + 2 = p + 2 \ . \qquad (22)$$

End of proof.

The Kochen-Specker subgraph lies behind a number of quantum "paradoxes". Thus, consider the Aharon-Vaidman game [11], in which Alice prepares a particle. She can place it in one of two boxes, or in none of them, and then hands the boxes to Bob. Bob is allowed to open one box to see if it contains the particle, and then leaves it as he found it. At the end of each run Alice is allowed to perform a measurement and can decide to cancel that particular run of the game. For all the runs that she decides to count, she wins if Bob found the particle. (There is an on-looker who ensures that Bob does not cheat.) The question is: can Alice select the runs that are counted in such a way that she always wins? Classically the answer is clearly "no", in particular the extra option of not placing the particle in any of the boxes is worse than useless for her. But Alice has studied the Kochen-Specker subgraph with some care. She prepares the particle in the state

$$|\psi_u\rangle = |\text{first box}\rangle + |\text{second box}\rangle + |\text{no box}\rangle \ . \qquad (23)$$

If Bob opens the first box and finds the particle, he leaves it in the state $|e_1\rangle = |\text{first box}\rangle$, if he does not find the particle in the first box he leaves it in the orthogonal state $|e_3\rangle = (|\text{second box}\rangle + |\text{no box}\rangle)$, and similarly if he opens the second box. At the end Alice makes a measurement corresponding to the projector $|\psi_d\rangle\langle\psi_d|$. If she gets the answer "yes" she knows that Bob found the particle.

Since Alice knows that Bob did open the box one can argue that her state assignment has changed to an appropriate density matrix, but since

she knows nothing about what Bob did or saw this does not change her probability to obtain "yes". This is still given by eq. (20), which means that she can select one ninths of all the runs in such a way that she always wins.

5. Hardy's paradox

Another interesting application of the Kochen-Specker subgraph is to Hardy's paradox [12], which has been translated into experiments [16]. The paradox concerns four dichotomic variables, the pair A_i controlled by Alice and the pair B_i controlled by Bob. It is assumed that

$$P(B_2 = 0|A_1 = 1) = P(A_2 = 0|B_1 = 1) = P(A_2 = 1, B_2 = 1) = 0 . \quad (24)$$

Hence it would seem that if A_1 and B_1 were both true, then A_2 and B_2 would both have to be true too, but this never happens in a single experiment. A paradox therefore arises when

$$P(A_1 = 1, B_1 = 1) \neq 0 . \quad (25)$$

But this logical structure is obtained by adding a single "outlier" to the Kochen-Specker subgraph; see Fig. 4 which also introduces some notation. All the states in the two pentagons except the upper vector $|a_1b_1\rangle$ are orthogonal to the outlier $|a_2b_2\rangle$. Therefore 7 of the 9 states in the graph lie in a three dimensional subspace. The state $|a_1b_1\rangle$ must have a component in this subspace so as to not coincide with the outlier, but it cannot be confined to it since $\langle a_1b_1|a_2b_2\rangle = 0$ would cause the construction to collapse.

This is very much a four dimensional paradox, since the entry of Alice and Bob requires the upper pentagram to be made of separable states only. The only vector in the graph which is not separable is $|\Psi\rangle$, the state that the system is actually in. But the outlier state $|a_2b_2\rangle$ ensures that all other states are uniquely determined by the upper pentagon, since all other states except $|a_1b_1\rangle$ are confined to three dimensions. As stressed by Penrose the logical structure is in a sense three dimensional [17].

The non-classical probability that we wish to maximise, under the constraint that all vectors in the graph except $|\Psi\rangle$ are separable, is
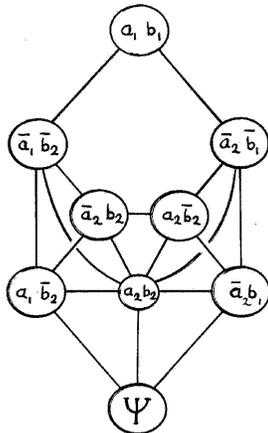
Figure 4: The orthogonality graph for Hardy's paradox; the notation is that "$a_1\bar{b}_2$" stands for the state where the eigenvalue of A_1 is 1 and the eigenvalue of B_2 is 0, etc. The orthogonalities enjoyed by the state $|\Psi\rangle$ ensure that eqs. (24) hold.

$$p = |\langle a_1 b_1 | \Psi \rangle|^2 \ . \tag{26}$$

The exact answer [18] is

$$p = \frac{1}{\Phi^5} \approx 0.09 \ . \tag{27}$$

Using the very same argument that led to eq. (22) we can show that maximising p is equivalent to maximising the amount by which $|\Psi\rangle$ violates the pentagram inequality for the upper pentagon in the graph.

6. Unfinished work and open questions

We did not complete the classification of all pentagrams in 4 dimensions. We can choose the pentagram vectors to be either maximally entangled (real, with $C = 1$) or separable ($C = 0$). We can still define a regular pentagram as one in which the scalar products between the non-orthogonal vectors have the same moduli. Among separable pentagrams the regular pentagram is unique, and has the eigenvalues

$$\vec{\lambda} = (2.148, 1.470, 1.240, 0.142) \ . \tag{28}$$

The maximal violation of the KS inequality is somewhat less than the largest violation in 3 dimensions. For maximally entangled (real) pentagrams, there are two regular solutions. One of them is simply the three dimensional regular pentagram with an extra zero eigenvalue added, the other has

$$\vec{\lambda} = (1.809, 1.809, 0.691, 0.691) \tag{29}$$

and does not lead to a violation. We note that there exists a set of 18 real vectors in 4 dimensions that are non-colourable, and lead to an absolute rather than probabilistic Kochen-Specker contradiction [19]. The corresponding orthogonality graph contains a pentagram subgraph [20] whose eigenvalues turn out to be

$$\vec{\lambda} = (2.171, 1.235, 1.5, 0.093) \ , \tag{30}$$

leading to a rather large violation.

The reader may wonder why we restrict ourselves to pentagons. Why not heptagons? In 3 dimensions the answer is simple: although there is a KS inequality associated to the heptagon, the maximal violation is smaller (in the precise sense that it is more sensitive to added noise [21]). It may be interesting to pursue heptagons in higher dimensions though.

Recently several experiments related to the Kochen-Specker theorem have been performed [22, 23, 24]. We would obviously be delighted to see an experimental violation of the pentagram inequality. The challenging part of such an experiment would be to verify that the Kochen-Specker rules apply in all cases where the theory says that they can be checked with simultaneous measurements.

We end on a speculative note. Take any Kochen-Specker graph in 3 or 4 dimensions leading to an absolute rather than a probabilistic Kochen-Specker contradiction, such as the one briefly alluded to above. Enumerate all its pentagram subgraphs. Is it by any chance the case that every vector in Hilbert space will violate at least one of the corresponding pentagram inequalities?

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