What is contextuality, and what is the principle of consistent exclusivity?

Marius Krumm, Fabian Lauble for the lecture
Quantum correlations and generalized probabilistic theories: an introduction
by Markus P. Müller at the University of Heidelberg

26th October 2014

1 Measurement results depend on the context of a measurement

[For details, see Peres' book [1] or [2]]
While Quantum Theory exists already for roughly 100 years, it still remains mysterious. For example, there is Quantum non-locality in the sense of a 'spooky action at distance' that is exhibited by entangled quantum systems.
Another puzzling property of the quantum world is called contextuality, which does not depend on special states such as entanglement. It is therefore more general but also needs stronger postulates.
Contextuality, like nonlocality, is a property that rules out classical hidden variable theories. Analogously to nonlocality, inequalities can be constructed from the classical assumption of noncontextuality that are violated by quantum theory, nature (experiments) and contextual correlations in general.
Contextuality refers to the property of a physical theory that a measurement's outcomes are not solely determined by the choice of the measured quantity and the measured system's (possibly hidden) state variables.

To make this statement more precise, we consider two plausible, i.e. classically motivated assumptions:

The first assumption is *independence of context*:
Consider three observables A, B, C with $[A, B] = [A, C] = 0$, e.g. $A = \vec{J}^2$, $B = J_x$, $C = J_z$. Thus A can be measured alone, or together with B or C. One would expect that the measurement outcome for A does solely depend on the measured system and its properties. Especially, one would expect that the measurement outcome for A does not depend on whether A is measured alone, together with B or together with C. This assumption allows to associate a value to A, which only depends on A.

The second assumption is *functional consistency*:
Consider two observables A, B that can be measured together, i.e. $[A, B] = 0$. Furthermore consider a function $f(\cdot, \cdot)$. $f(A, B)$ can be measured together with A and B and the measurement outcomes for A, B and $f(A, B)$ should have the same functional relationship as the operators: If we measure a for A, b for B, then we should get $f(a, b)$ for $f(A, B)$, no matter which state we use. Even if the measurement is

not actually performed, one would also expect the numerical measurement results (if the measurement was performed) to fulfill the same relationship as the operators, i.e. if a is the value for A and b the value for B, $f(a,b)$ should be the value for $f(A,B)$.

The two reasonable assumptions of *independence of context* and *functional consistency* are incompatible with quantum theory when taken together. Consider a pair of spin 1/2 particles in any state. These 9 nicely arranged operators

$$\begin{array}{ccc} \mathbb{1} \otimes \sigma_z & \sigma_z \otimes \mathbb{1} & \sigma_z \otimes \sigma_z \\ \sigma_x \otimes \mathbb{1} & \mathbb{1} \otimes \sigma_x & \sigma_x \otimes \sigma_x \\ \sigma_x \otimes \sigma_z & \sigma_z \otimes \sigma_x & \sigma_y \otimes \sigma_y \,, \end{array} \tag{1.1}$$

on a two-qubit Hilbert space consisting of the three Pauli matrices and the identity, have the following properties: All operators have eigenvalues ± 1, the operators in each column and each row commute and any operator is the product of the other two operators in the same row/column, *except* for the last column, i.e.:

$$(\sigma_x \otimes \sigma_z)(\sigma_z \otimes \sigma_x) = \sigma_y \otimes \sigma_y \qquad (\sigma_z \otimes \sigma_z)(\sigma_x \otimes \sigma_x) = -\sigma_y \otimes \sigma_y \tag{1.2}$$

By independence of context, we will assume that we can assign a value to every operator without caring for the chosen measurement. As these values are supposed to be the measurement outcomes, if the measurements were actually performed, they have to be eigenvalues (i.e. ± 1). We assign values called $a, b, c, d \in \{\pm 1\}$ to the 4 operators in the upper left corner of (1.1). Afterwards we use functional consistency to find the values of the operators in the third column and the third row:

$$\begin{array}{cccc} a & b & \rightarrow & ab \\ c & d & \rightarrow & cd \\ \downarrow & \downarrow & & \downarrow \\ & & & -abcd \\ ac & bd & \rightarrow & +acbd \end{array} \tag{1.3}$$

As one can see, the additional minus sign in the third column leads to a contradition.

The assumptions together therefore contradict quantum theory. Therefore, (self-consistent) measurement results have to depend on the exact context of a measurement, not just the system and the measured property.

2 Exclusivity

> *"The fundamental theorem of QM [might be that] if you have several questions and you can answer any two of them [i.e., if the corresponding propositions (or events) are pairwise decidable], then you can also answer all of them" [i.e., the corresponding propositions are simultaneously (or jointly) decidable]*
>
> — Ernst Specker, after having a piece of cake [3]

[For details, see [4]]
Analogously to non-locality which violates Bell type inequalities (CHSH for example), contextual theories violate inequalities such as the KCBS (Klyachko-Can-Binicioğlu-Shumovsky) inequality. Quantum theory's violation of Bell inequalities is bounded (recall *Tsirelson's bound* $\leq 2\sqrt{2}$ for CHSH) and an upper bound for more general theories, the non-signalling ones, also exists (≤ 4 for CHSH). Intense research has been undertaken to find underlying principles for Tsirelson's bound.
Similar studies can be made for the KCBS inequality. In the following, $a, b, c, d|w, x, y, z$ indicate the event that the compatible tests w, x, y, z were performed and that the respective results a, b, c, d have been obtained. Two events $a_1, a_2, \ldots |w_1, w_2, \ldots$ and $a'_1, a'_2, \ldots |w'_1, w'_2, \ldots$ are called *exclusive* if any outcomes for the same test are different: $\exists\ j, k : w_j = w'_k$ but $a_j \neq a'_k$

The principle of *(consistent) exclusivity* is that the sum of the probabilities of pairwise exclusive events cannot exceed 1. This is not as trivial as it may sound since the considered probabilities $P(a, b, c, d|w, x, y, z)$ are *conditional* probabilities, their context (the other tests) is taken into account.
As Cabello said, "*[t]his principle follows from Specker's observation that pairwise decidable events must not necessarily be jointly decidable, and from Boole's axiom of probability stating that the sum of the probabilities of events that are jointly exclusive cannot exceed* 1." [4]
Consider the events $a, b|x, y$ with $a, b \in 0, 1,\ x, y \in 0, 1, 2, 3, 4$. The KCBS inequality for non-contextual hidden variable theories (NCHV) reads

$$\sum_{i=0}^{4} P(0, 1|i, i+1) \overset{\text{NCHV}}{\leq} 2 \overset{\text{QM}}{\leq} \sqrt{5} \overset{E}{\leq} \frac{5}{2} \tag{2.4}$$

Here, the sum is taken modulo 5, $\sqrt{5}$ is the maximum quantum violation and $5/2$ is the maximum violation of theories compatible with exclusivity. It is not difficult to understand the maximum violation respecting (consistent) exclusivity. Consider the five events

$$\begin{gathered}(0, 1|0, 1)\\(0, 1|1, 2)\\(0, 1|2, 3)\\(0, 1|3, 4)\\(0, 1|4, 0)\end{gathered}$$

that are considered in the inequality. Swapping the places of measurement *and* outcome in every other event, the set is (in the same order)

$$\begin{gathered}(0, 1|0, 1)\\(1, 0|2, 1)\\(0, 1|2, 3)\\(1, 0|4, 3)\\(0, 1|4, 0)\,.\end{gathered}$$

It is now clear that the event pairs $(1,2)$, $(2,3)$, $(3,4)$ and $(4,5)$ are exclusive. Swapping the digits in the first event, one also sees that the event pair $(1,5)$ is exclusive. One can therefore arrange the events in a pentagonal shape where every pair of adjacent vertices represents a pair of exclusive events (see fig. 2.1).

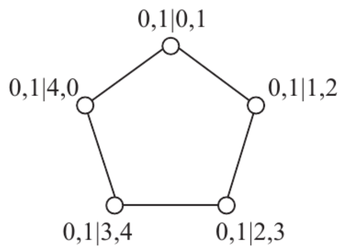

Figure 2.1: *This figure shows the 5 events considered in the exclusivity-scenario. Events that are exclusive are connected by a straight line. This figure is an example for a graph: The events are represented by vertices, the lines connecting exclusive events are called edges. Taken from [4].*

According to the principle of (consistent) exclusivity, the sum of probabilities of every such pair is ≤ 1. We can therefore rewrite the sum of the five probabilities

$$\sum_{i=0}^{4} P(0,1|i,i+1) = \frac{1}{2}\sum_{i=0}^{4} 2P(0,1|i,i+1) = \tag{2.5}$$

$$\frac{1}{2}\sum_{i=0}^{4}\Big[\underbrace{P(0,1|i,i+1) + P(0,1|i+1,i+2)}_{\leq 1}\Big] \overset{\mathrm{E}}{\leq} \frac{1}{2}\sum_{i=0}^{4} 1 = \frac{5}{2}, \tag{2.6}$$

which is the upper bound for theories respecting (consistent) exclusivity.

Cabello derived [4] [5] the maximum quantum violation from a property called *global exclusivity*. The principle is global in the sense that two separate KCBS experiments are considered, for example one in Stockholm and one in Vienna, possibly space-like separated. Local events in Vienna are denoted by $0,1|i_{\mathrm{V}}, i+1_{\mathrm{V}}$ while events in Stockholm are denoted by $0,1|j_{\mathrm{S}}, j+1_{\mathrm{S}}$. The combined, 'global' events are written as $0,1,0,1|i_{\mathrm{V}}, i+1_{\mathrm{V}}, j_{\mathrm{S}}, j+1_{\mathrm{S}}$ (see figure (2.2)). Exclusivity of two local events is inherited by the global events (since one contradicting result suffices), so starting from sets of five events with pentagon-shape exclusivity per city, we get a set of 5 *pairwise* exclusive global events

$$\begin{aligned}
&0,1,0,1|i_{\mathrm{V}}, i+1_{\mathrm{V}}, j_{\mathrm{S}}, j+1_{\mathrm{S}}\\
&0,1,0,1|i+1_{\mathrm{V}}, i+2_{\mathrm{V}}, j+2_{\mathrm{S}}, j+3_{\mathrm{S}}\\
&0,1,0,1|i+2_{\mathrm{V}}, i+3_{\mathrm{V}}, j+4_{\mathrm{S}}, j_{\mathrm{S}}\\
&0,1,0,1|i+3_{\mathrm{V}}, i+4_{\mathrm{V}}, j+1_{\mathrm{S}}, j+2_{\mathrm{S}}\\
&0,1,0,1|i+4_{\mathrm{V}}, i_{\mathrm{V}}, j+3_{\mathrm{S}}, j+4_{\mathrm{S}}.
\end{aligned}$$

Five independent such sets (for different choice of j) exist. Here Vienna ensures exclusivity of adjacent vertices and Stockholm ensures exclusivity on the 'diagonals' of the pentagon. Therefore, these 5 events are pairwise exclusive. The sum of their probabilites is therefore ≤ 1 according to the principle of exclusivity:

$$\sum_{i=0}^{4} P(0,1,0,1|i_{\mathrm{V}}, i+1_{\mathrm{V}}, j+2i_{\mathrm{S}}, j+2i+1_{\mathrm{S}}) \leq 1\,.$$

The notation with $+2i$ (modulo 5) gives precisely 5 events as considered above. Since the index j is left open, 5 such sets exist. Summing over j, the probability of all 25 global events reads

$$\sum_{j=0}^{4}\sum_{i=0}^{4} P(0,1,0,1|i_{\mathrm{V}}, i+1_{\mathrm{V}}, j+2i_{\mathrm{S}}, j+2i+1_{\mathrm{S}}) \leq 5\,.$$

Since the two experiments in Stockholm and Vienna are independent, the probability factorizes:

$$\sum_{i=0}^{4}\left[P(0,1|i_{\mathrm{V}}, i+1_{\mathrm{V}})\left(\sum_{j=0}^{4} P(0,1|j+2i_{\mathrm{S}}, j+2i+1_{\mathrm{S}})\right)\right] \leq 5\,.$$

The sum of the probabilities of the local events in Stockholm is not affected by the $+2i$ term as this only changes the order of summing. We therefore arrive, with a change of indices, at

$$\left(\sum_{i=0}^{4} P(0,1|i_{\mathrm{V}}, i+1_{\mathrm{V}})\right)\left(\sum_{l=0}^{4} P(0,1|l_{\mathrm{S}}, l+1_{\mathrm{S}})\right) = \left(\sum_{k=0}^{4} P(0,1|k,k+1)\right)^2 \leq 5\,,$$

□

which gives the maximum quantum violation $\sqrt{5}$ of the KCBS inequality (2.4).

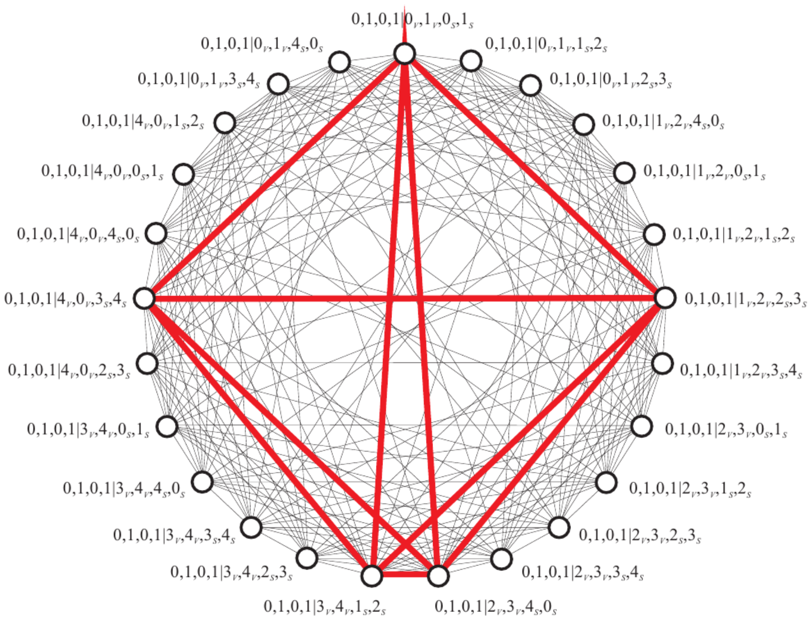

Figure 2.2: *This figure shows the 25 events considered in the global exclusivity scenario. Pairwise exclusive events are connected by black lines. Also shown are 5 events which are pairwise exclusive; they are connected by red lines. Taken from [4].*

3 Graph theoretic formalisation

[For details, see [6]]
We have already seen in the previous chapter, that it can be helpful to use graphs consisting of vertices and edges to visualise events and their relations. There has been successful research about the connection of graph theoretic numbers and inequality-violation boundaries, some examples are mentioned in [4]. Therefore it is natural to use graph theory to develop a framework which allows to discuss contextuality and exclusivity in a formal way.

Definition 1. *A **graph** is an ordered pair $G = (V, E)$ comprising a set V of vertices or nodes together with a set E of edges or lines, which are 2-element subsets of V (i.e., an edge is related with two vertices, and the relation is represented as an unordered pair of the vertices with respect to the particular edge).[7]*

An example for a graph is given by fig. (2.1).

Definition 2. *A **hypergraph** is a generalisation of a graph in the sense that not only 2-element subsets of V are allowed as edges but any subsets.*

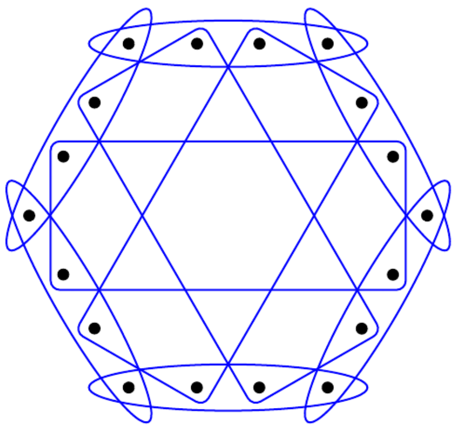

Figure 3.1: *This figure shows an example for a hypergraph. Edges are represented not by lines, but by blue bubbles. The reason for this is, that edges in a hypergraph can contain more than two elements. Taken from [6].*

Definition 3. *A **contextuality scenario** is a hypergraph H with set of vertices $V(H)$ and set of edges $E(H) \subset \boldsymbol{P}(V(H))$ [1] such that $\bigcup_{e \in E(H)} e = V(H)$.*

"*We think of the edges as all the possible measurements which can be conducted on a system. A consistent measurement statistic will assign a probability to each outcome, in such a way that the total probability for each measurement is 1.*" [6] Thus one defines:

Definition 4. *Let H be a contextuality scenario. A **probabilistic model** on H is an assignment $p : V(H) \to [0, 1]$ of probabilities $p(v)$ to each vertex such that*

$$\sum_{v \in e} p(v) = 1 \quad \forall e \in E(H) \tag{3.7}$$

[1]The *power set* $\boldsymbol{P}(S)$ of a set S is the set of all subsets of S, including the empty set $\emptyset$ and S itself.

For any Hilbert space $\mathcal{H}$, we call $B(\mathcal{H})$ the set of (bounded) operators and $B_+(\mathcal{H})$ the set of positive semi-definite (hermitian) operators. $B_{+,1}(\mathcal{H}) := \{\rho \in B_+(\mathcal{H}) | \mathrm{Tr}(\rho) = 1\}$.

Definition 5. *Let H be a contextuality scenario. An assignment of probabilities $p : V(H) \to [0,1]$ is a* ***quantum model*** *if there exists a Hilbert space $\mathcal{H}$, a quantum state $\rho \in B_{+,1}(\mathcal{H})$ and a projection operator[2] $\mathcal{P}_v \in B(\mathcal{H})$ associated to every $v \in V(H)$ which constitute projective measurements in the sense that*

$$\sum_{v \in e} \mathcal{P}_v = \mathbb{1} \quad \forall e \in E(H) \tag{3.8}$$

and reproduce the given probabilities,

$$p(v) = \mathrm{Tr}(\rho \mathcal{P}_v) \quad \forall\, v \in V(H). \tag{3.9}$$

Remark: We only consider finite-dimensional Hilbert spaces.

Definition 6. *A probabilistic model p satisfies* ***Consistent Exclusivity*** *if*

$$\sum_{v \in I} p(v) \leq 1 \tag{3.10}$$

holds for any $I \subseteq V(H)$ a set of vertices in a contextuality scenario H such that every two of them belong to a common edge.

We will now show that Quantum Theory as a probabilistic model satisfies Consistent Exclusivity (see Theorem 1).

Lemma 1. *Consider a Quantum Model. Let $\{\mathcal{P}_v | v \in e\}$ be a set of projectors of an edge, especially $\sum_{v \in e} \mathcal{P}_v = \mathbb{1}$. Then $\mathcal{P}_w \mathcal{P}_v = 0$ for $v \neq w$ where $v, w \in e$.*

Proof. Assume $v \neq w \in e$. Let $|n_v\rangle$ be an eigenstate of $\mathcal{P}_v$. As $\mathcal{P}_v$ is a projector, the eigenvalues are 0,1. So if $\mathcal{P}_v |n_v\rangle = 0$, we find $\mathcal{P}_w \mathcal{P}_v |n_v\rangle = 0$. So let us assume now that $\mathcal{P}_v |n_v\rangle = |n_v\rangle$.

$$|n_v\rangle = \mathbb{1} |n_v\rangle = \sum_{v' \in e} \mathcal{P}_{v'} |n_v\rangle = |n_v\rangle + \sum_{v' \in e, v' \neq v} \mathcal{P}_{v'} |n_v\rangle \tag{3.11}$$

Thus $\sum_{v' \in e, v' \neq v} \mathcal{P}_{v'} |n_v\rangle = 0$, especially $\sum_{v' \in e, v' \neq v} \langle n_v | \mathcal{P}_{v'} |n_v\rangle = 0$. As the projectors are positive semi-definite, i.e. $\langle n_v | \mathcal{P}_{v'} |n_v\rangle \geq 0$, this requires $\langle n_v | \mathcal{P}_{v'} |n_v\rangle = 0$ for $v' \neq v$. Thus $\langle n_v | \mathcal{P}_w |n_v\rangle = 0$.
Let $\{|j_w\rangle\}$ be an orthonormal eigenbasis of $\mathcal{P}_w$, ordered such that $\mathcal{P}_w |j_w\rangle = |j_w\rangle$ for $j \leq m$ and $\mathcal{P}_w |j_w\rangle = 0$ for $j > m$ and expand $|n_v\rangle = \sum_{j=1}^{N} a_{nj} |j_w\rangle$ where N is the dimension of the Hilbert space. Then

$$0 = \langle n_v | \mathcal{P}_w |n_v\rangle = \sum_{j,k=1}^{N} a_{nj}^* a_{nk} \langle j_w | \mathcal{P}_w |k_w\rangle = \sum_{k=1}^{m} \sum_{j=1}^{N} a_{nj}^* a_{nk} \langle j_w | k_w\rangle = \sum_{j=1}^{m} |a_{nj}|^2 \tag{3.12}$$

[2]When using the term *projection operator*, we mean operators $\mathcal{P}$ with $\mathcal{P}^2 = \mathcal{P}$ and $\mathcal{P}^\dagger = \mathcal{P}$, i.e. orthogonal projection operators. So they have an orthonormal eigenbasis and only 0 and 1 as possible eigenvalues.

Thus $a_{nj} = 0$ for $j \leq m$. Therefore

$$\mathcal{P}_w |n_v\rangle = \sum_{j=1}^{N} a_{nj} \mathcal{P}_w |j_w\rangle = \sum_{j=1}^{m} a_{nj} |j_w\rangle = 0 \tag{3.13}$$

Especially, $\mathcal{P}_w \mathcal{P}_v |n_v\rangle = \mathcal{P}_w |n_v\rangle = 0$.

We have found that $\mathcal{P}_w \mathcal{P}_v |n_v\rangle = 0$ on a basis, i.e. $\mathcal{P}_w \mathcal{P}_v = 0$. □

Theorem 1. *Consider a Quantum model. Let* $\{\mathcal{P}_v | v \in I\}$ *be a collection of operators which pairwise belong to the same edge. Then* $\sum_{v \in I} \mathcal{P}_v \leq \mathbb{1}$*, i.e. quantum models satisfy consistent exclusivity.*

Proof. As every pair of the projectors share an edge, $\mathcal{P}_v \mathcal{P}_w = 0 \; \forall v \neq w \in I$, especially $[\mathcal{P}_v, \mathcal{P}_w] = 0$. So there exists a common orthonormal eigenbasis $|n\rangle$ of all the projectors. We write

$$\mathcal{P}_v |n\rangle = p_{vn} |n\rangle \tag{3.14}$$

where $p_{vn} \in \{0, 1\}$ is an eigenvalue.

Now assume $p_{vn} = 1$. Then $p_{wn} = 0 \; \forall w \neq v$:
$p_{wn} |n\rangle = \mathcal{P}_w |n\rangle = \mathcal{P}_w \cdot 1 |n\rangle = \mathcal{P}_w \cdot p_{vn} |n\rangle = \mathcal{P}_w \mathcal{P}_v |n\rangle = 0$ by the previous lemma.

Let $|\psi\rangle = \sum_n a_n |n\rangle$ be an arbitrary normalised state. Then

$$\langle\psi| \sum_{v \in I} \mathcal{P}_v |\psi\rangle = \sum_{j,k,v} a_j^* a_k \langle j| \mathcal{P}_v |k\rangle = \sum_{j,k,v} a_j^* a_k p_{vk} \langle j|k\rangle = \sum_{j,v} |a_j|^2 p_{vj} \tag{3.15}$$

$$= \sum_j |a_j|^2 \Big[\sum_v p_{vj}\Big] \leq \sum_j |a_j|^2 = \langle\psi|\psi\rangle = 1 \tag{3.16}$$

Thus $\sum_{v \in I} \mathcal{P}_v \leq \mathbb{1}$.

Thus with an orthonormal eigenbasis of ρ, $\rho |j_\rho\rangle = \lambda_j |j_\rho\rangle$:

$$\sum_{v \in I} p(v) = \mathrm{Tr}(\rho \sum_{v \in I} \mathcal{P}_v) = \sum_j \lambda_j \langle j_\rho| \sum_{v \in I} \mathcal{P}_v |j_\rho\rangle \tag{3.17}$$

$$\leq \sum_j \lambda_j \langle j_\rho| \mathbb{1} |j_\rho\rangle = \sum_j \lambda_j = \mathrm{Tr}\,\rho = 1 \tag{3.18}$$

□

4 Conclusion

In this paper, we summarized some results about a surprising quantum phenomenon called contextuality. At first, we presented a simple example from [1]/[2], which shows that self-consistent measurement outcomes necessarily depend on the context of the measurement. Afterwards we presented a result by Cabello[4], how a principle called global exclusivity leads to the maximum quantum violation of the KCBS-inequality. At last we summarised a graph theoretic formalisation from [6] which allows to discuss contextuality and (consistent) exclusivity.

References

[1] A. Peres, *Quantum Theory: Concepts and Methods*. Vol. 57, Kluwer Academic Publishers, 1993

[2] N. D. Mermin, *Simple Unified Form for the Major No-Hidden-Variables Theorems*, Phys. Rev. Lett. **65** (1990) 3373

[3] E. Specker. `http://vimeo.com/52923835`

[4] A. Cabello. *Simple Explanation of the Quantum Violation of a Fundamental Inequality.* Phys. Rev. Lett. **110** (2012), 060402. arXiv:1210.2988

[5] The version of the proof presented here was sent to us by the lecturer Markus P. Müller via private communication.

[6] A. Acín, T. Fritz, A. Leverrier and A.B. Sainz. *A Combinatorial Approach to Nonlocality and Contextuality*, arXiv:1212.4084

[7] Wikipedia (en): Graph (mathematics), 2014-09-21