INTER-FACULTY MASTER PROGRAM on
COMPLEX SYSTEMS and NETWORKS
SCHOOL of MATHEMATICS
SCHOOL of BIOLOGY
SCHOOL of GEOLOGY
SCHOOL of ECONOMICS
ARISTOTLE UNIVERSITY of THESSALONIKI

Master Thesis

Title:

Quantum Contextuality and Locality

Κβαντικό Πλαίσιο και Τοπικότητα

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ΔΙΑΤΜΗΜΑΤΙΚΟ ΠΡΟΓΡΑΜΜΑ ΜΕΤΑΠΤΥΧΙΑΚΩΝ ΣΠΟΥΔΩΝ στα
ΠΟΛΥΠΛΟΚΑ ΣΥΣΤΗΜΑΤΑ και ΔΙΚΤΥΑ
ΤΜΗΜΑ ΜΑΘΗΜΑΤΙΚΩΝ
ΤΜΗΜΑ ΒΙΟΛΟΓΙΑΣ
ΤΜΗΜΑ ΓΕΩΛΟΓΙΑΣ
ΤΜΗΜΑ ΟΙΚΟΝΟΜΙΚΩΝ ΕΠΙΣΤΗΜΩΝ
ΑΡΙΣΤΟΤΕΛΕΙΟ ΠΑΝΕΠΙΣΤΗΜΙΟ ΘΕΣΣΑΛΟΝΙΚΗΣ

Μεταπτυχιακή Διπλωματική Εργασία

Τίτλος Εργασίας:

Κβαντικό Πλαίσιο και Τοπικότητα

Quantum Contextuality and Locality

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ΕΠΙΒΛΕΠΩΝ: Αντωνίου Ιωάννης, Καθηγητής
Τμήματος μαθηματικών, Α.Π.Θ

Εγκρίθηκε από την Τριμελή Εξεταστική Επιτροπή την 17η Δεκεμβρίου 2019.

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Θεσσαλονίκη, Δεκέμβριος 2019

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Ευχαριστίες

Ολοκληρώνοντας την φοίτησή μου στο Δ.Π.Μ.Σ στα Πολύπλοκα Συστήματα και Δίκτυα του Α.Π.Θ, θα ήθελα να ευχαριστήσω από καρδιάς όλους αυτούς τους ανθρώπους που στάθηκαν δίπλα μου και με βοήθησαν, ο καθένας ξεχωριστά και με τον δικό του τρόπο, να φέρω σε πέρας τις σπουδές μου και να ολοκληρώσω την παρούσα εργασία.

Πρώτον απ' όλους θα ήθελα να ευχαριστήσω τον επιβλέποντα καθηγητή μου, κ. Αντωνίου, όχι μόνο για τις πολλές γνώσεις που μοιράστηκε μαζί μου, αλλά και για την υπομονή που επέδειξε για τον ιδιαίτερο τρόπο που σκέφτομαι και μελετάω. Θα ήθελα επίσης να ευχαριστήσω τους γονείς μου, Θωμά και Κατερίνα, καθώς και την κοπέλα μου Χρύσα, για την αγάπη τους και την συνεχή ψυχολογική τους στήριξη. Τέλος, θέλω να ευχαριστήσω τους φίλους μου Πέτρο, Γιάννη, Σίμο, Ιωάννα και Ξενοφώντα, για τις συμβουλές, την βοήθεια, και κυρίως την παρέα τους.

«Η διπλωματική εργασία είναι αφιερωμένη στην θεία μου Ελισσάβετ, τον πρώτο άνθρωπο που με δίδαξε μαθηματικά».

Περίληψη

Στην παρούσα διπλωματική εργασία θα μελετήσουμε τις έννοιες του κβαντικού πλαισίου και της τοπικότητας. Αρχικά θα υπάρξει μία παρουσίαση των εννοιών η οποία θα ακολουθηθεί από μια παρουσίαση των σημαντικότερων θεωρημάτων σχετικών με το θέμα, δηλαδή του θεωρήματος του Bell και του θεωρήματος του Kochen και Specker. Κατόπιν, θα προσεγγίσουμε τις προαναφερθείσες έννοιες από την σκοπιά της θεωρίας γράφων, και θα συνεχίσουμε υποδεικνύοντας τα σημαντικότερα συμπεράσματα και προϋποθέσεις γύρω από την ύπαρξη της τοπικότητας και των πλαισιακών σχέσεων. Τέλος, θα μελετήσουμε τις μονογαμικές σχέσεις που δύνανται να εμφανιστούν ανάμεσα στις ανισότητες ανίχνευσης μη-τοπικών και πλαισιακών φαινομένων, και θα παρουσιάσουμε μερικά ενδιαφέροντα παραδείγματα και εφαρμογές που εκμεταλλεύονται τις παραπάνω μονογαμικές σχέσεις.

Abstract

In this master thesis we are going to study the concepts of contextuality and locality. At first there is a presentation of the notions of locality and quantum contextuality, followed by the presentation of the most important theorems related to the subject, namely the Bell theorem and the Kochen-Specker theorem. Afterwards, we will approach the notions of locality and contextuality from a graph-theoretical point of view, and we will proceed by showing some important statements and conditions about them. Finally, we are going to study the monogamous relations that may appear between the corresponding local and non-contextual test inequalities, and we will present some interesting examples and applications that utilize the aforementioned monogamous relations.

Contents

0 Prologue

The discovery of the quantum nature of light and subatomic particles changed decidedly the way we perceive the world. Suddenly, we realized that our understanding about the fundamental laws of the universe was far from the realistic, and that the solid theoretical structure we have created in order to study the world around us, started to rumble. Many philosophical discussions and scientific debates took place until the first concrete theories, which would allow us to acquire answers through experimental methods, to appear. The counterintuitive explanations that the Quantum theory provided, made it one of the most well tested physical theories in the history of science. From the very beginning of its formulation, many leading scientists at the time had serious objections about the rightness of the theory. Therefore, the study of the fundamental principles that underlie the quantum theory has become one of the most important topics for research in these days.

1 Locality

1.1 About the EPR Paradox

When the Quantum Mechanics theory initially formulated, many scientists considered that the explanation of physical reality provided by Quantum Theory was incomplete. In a 1935 paper [Einstein et al 1935] Einstein, Podolsky and Rosen proposed a thought experiment in order to show that the wave function does not contain complete information about physical reality, and hence the Copenhagen interpretation is unsatisfactory. The original EPR paradox questions the predictions of quantum theory, given that it is impossible to know both the position and the momentum of a quantum particle.

The EPR argument is the following [EPR 1935, Kumar 2011]: Let two particle systems I and II interact and then separated with each other, so they can be in an "entangle state" in which measuring particle's I position or momentum predicts particle's II position or momentum respectively and vice versa. This is a case which quantum theory clearly allows. As the Heisenberg's uncertainty principal states, it is impossible to measure to measure both the exact momentum and exact position of a specific particle. Now, let us consider Alice who makes measurements on system I, and Bob who makes measurements on the remote isolated system II. If Alice measures the exact position of particle I, she can work out immediately the exact position of particle II. Alternatively, if Alice decides to measure the exact momentum of particle I, she can immediately derive the exact momentum of Bob's particle. Consequently, the particle II would have simultaneously exact values of position and momentum, something that is impossible according to Heisenberg's principle. Therefore, the Einstein, Podolsky and Rosen, conclude that the Quantum mechanical description of physical reality given by wave functions is not complete.

In order to resolve the paradox, Einstein, Podolsky and Rosen proposed the existence of a more "complete" theory which contains variables corresponding to "all elements of reality". In that theory, "Hidden Variables" that are inaccessible to us, provide a way to account for all observable behavior and thus avoid indeterminism. The Hidden Variables theories [Wheeler, Zurek 2014] are deterministic theories in opposition to the fundamental probabilistic nature of the Quantum Mechanics (QM).

This is a good point to note something about the assumptions made by the EPR. In order to construct this thought experiment, Einstein, Podolsky and Rosen made a crucial assumption: by simply measuring particle I, Alice does not disturb or influences particle II, which, after all, can be far away and isolated from influences of the rest of the universe. They took this argument as perfectly normal case of scientific common-sense reasoning applied in a specific theory. But the story does not end here. In 1964 John Bell [Bell, 1964] realized that if the "local-realistic" assumption of EPR holds, an actual experiment would give different results from the case in which a non-local correlations theory holds.

1.2 What is the relation between Locality, Realism and Bell Inequalities?

In physics, "local realism" [Clauser, Shimony 1978] is the belief that the physical world exists independently of any possible observer, and that any physical effect can be described as an interaction of any distinct point with its direct neighboring points. Essentially, local realism is the combination of the principle of Locality with the assumption of realism.

As mentioned above, the principle of locality states that an object is directly influenced only by its immediate surroundings. This principle seems to be a very natural and reasonable conclusion that anyone who studies classic physics could end up with. A physical theory that includes the principle of locality is said to be a "local theory". Locality has evolved out of the field theories of classical physics, and has a close relation with the special theory of relativity, which limits the propagation speed of all possible information to the speed of light.

On the other hand, Realism, in the sense of physics, [Norven 2007] is the idea that nature exists independently of the observer. However, the notion of realism is not well defined or globally accepted, and many scientists consider the use of term "Outcome Determinism" (OD) [Stanford Encyclopedia of Philosophy] as a more suitable notion for describing the essence of the argument. Outcome Determinism stating that the "hidden state" λ uniquely determines the outcome of any experiment, and quantum uncertainty relations are due to our inability to specify those states. The conditional probabilities $p\,(x^a, y^b|\lambda)$ take the extremal values 0 or 1.

$$\forall\lambda, a, b \;\; \& \;\; \forall x^a \in X_A, \forall y^b \in Y_B, \;\; p\,(X^a = x^a, Y^a = y^a|\Lambda = \lambda) \in \{0,1\} \qquad \text{(OD)}$$

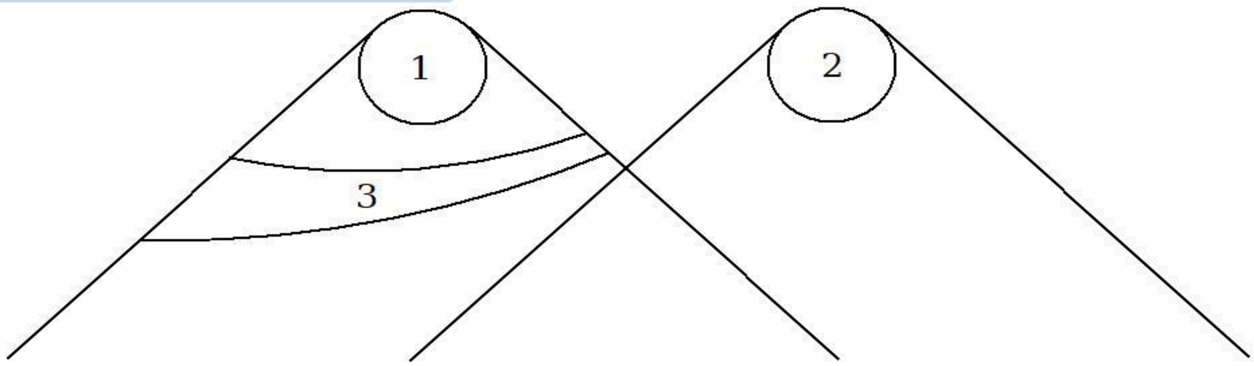
However, with the formulation of the Quantum theory some cases arose that seemed to defy the principle of local realism. Many scientists considered that a Hidden Variable (HV) model would be a more suitable theory for explaining the physical evidence than the Copenhagen interpretation which supported the probabilistic nature of quantum mechanics. The basic concept of a hidden variable model is the existence of a value λ which contains the entirety of the properties of the system. By defining the variable space Λ which is the totality of all possible values λ, a HV theory assumes the existence of a probability distribution $\rho(\lambda)$ of the hidden states of Λ and the existence of joint probability distribution $p\left(x^{\vec{s}}|\lambda\right)$ for every $\lambda \in \Lambda$, which gives the probability of the $x^{\vec{s}}$ to be the experimental outcome result given that the system is in hidden state λ and the measurement settings are $\vec{s}$.

In 1964 John Bell, in order to derive an inequality that will distinguish local from non-local effects, made an assumption known as "Factorizability condition" (F) or as "Bell locality" [Bell 1981], which every HV model should satisfy. Let us consider the case of a pair of physical systems labeled as 1 and 2. The Factorizability condition states that if each pair of systems is characterized by a hidden value λ, then for any measurement settings a, b on the systems 1 and 2 respectively, and for every $\lambda \in \Lambda$, there exist probability functions $p_1(x^a|\lambda)$, $p_2(y^b|\lambda)$, such that $p\,(x^a, y^b|\lambda) = p_2(x^a|\lambda)\, p_2(y^b|\lambda)$, where x and y be the measurement results for systems 1 and 2 respectively. Bell derived the Factorizability condition from a condition he called "Principle of Local Causality" [Norsen 2011]. Principle of Local Causality states the following:

"The direct causes and effects of events are nearby, and even the indirect causes and effects are no further away than permitted by the velocity of light."

Because the previous statement is not suitable for a more mathematical description of the theory, Bell introduced a "sharpened" version of the principal:

A theory will be said to be locally causal if the probabilities attached to values of a physical theory's elements that corresponds to something physically real contained within a space-time region 1 are unaltered by specifications of values on other elements of the same physical theory within a space-like separated region 2, when what happens in the backward light cone of 1 is already sufficient specified, for example by a full specification of physical theory's elements contained within a space-time region 3 [Stanford Encyclopedia of Philosophy].



Summarizing, a HV theory assumes the existence of a complete state space Λ that completely determines the results of any experiment with given settings, and satisfies the conditions of Factorizability (locality), and Outcome Determinism (realism). Bell, considering these two assumptions manage to derive a no-go theorem in order to examine if a hidden variable theory is a valid case for quantum mechanics. He generated an inequality and proved that if a HV theory governs the quantum mechanics, this inequality should be satisfied. If on the other hand, there was a case in which the inequality is defied, at least one of the assumptions of Outcome determinism or Factorizability must be wrong.

In this point, we should mention two interesting theorems:

1.2.1 Theorem (Suppes, Zanotti 1976)

> For the special case of perfect correlations between outcomes of the two experiments, that is when the outcome of an experiment in one system determines completely the outcome of the experiment in the other, (OD) condition must be satisfied if the (F) condition is.

This theorem applies to the specific case Bell considered in 1964, in which the two systems was perfectly anti-correlated. Although (OD) is not generally being assumed, the theorem below shows that we could assume it.

1.2.2 Theorem (Fine 1982)

The following are equivalent:

1. There is a deterministic HV model.

2. There is a factorizable, stochastic model.
3. There is one joint distribution for all observables, returning the experimental probabilities.
4. There are well-defined, compatible joint distributions for all pairs and triples for commuting and non-commuting observables.
5. The Bell inequalities hold.

From the theorems above we can conclude that the Locality (F), the Outcome Determinism (OD), the existence of a joint distribution of all observables and the satisfaction of Bell inequalities, are equivalent notions.

1.3 Bell theorem

In 1964, John Bell, in order to provide a way to distinguish local-realistic from non-local-realistic effects, formulated a framework and derived an inequality that indicates non-local-realistic correlations. More precisely, when Bell's inequality is defied, we observe a non-local effect. In the present section we will show a proof of a No-go theorem of Bell's type as presented in the Stanford Encyclopedia of Philosophy.

For the construction of the conceptual framework consider an ensemble of pairs of systems, with the individual systems in each pair being labeled as 1 and 2. Different experiments may be performed on each system. Let us call the variables that describe the experiment settings on system 1 as a, a' and the variables of the experiment settings on system 2 as b and b'. It is not assumed that these parameters capture the complete state of the experimental apparatus. We denote with x the result of an experiment, performed with some setting a, on system 1, which furthermore takes values from a discrete set X_a of real numbers in the interval $[-1,1]$. Likewise, we denote with y the result of an experiment on system 2 with some setting b, which also takes values from a discrete set Y_b in the interval $[-1,1]$. The sets of potential outcomes may depend on the experimental settings. Also, note that the restriction of the values of the outcome labels is of no physical significance, and is a choice made only for convenience. Bell's original version of the theorem assumed experiments with only two possible outcomes labeled ± 1.

Assuming that a Local Hidden Variable theory is a valid case, the following conditions should be satisfied:

1. There is a hidden variable space Λ, which is the collection of all the possible hidden values λ. The hidden values λ contain the entirety of the properties of the system at the moment of generation and remain inaccessible to observers.
2. We have an appropriate choice of subsets of Λ to be regarded as the measurable subsets, forming a measurable space to which probabilistic considerations may be applied. That considerations are that:
   a. There is a normalized distribution ρ of Λ with $\int_{\Lambda} \rho(\lambda)\, d\lambda = 1$.
   b. For every pair of settings a, b and every $\lambda \in \Lambda$ there is a probability function $p\,(x^a, y^b|\lambda)$ which take values in the interval $[0,1]$ and satisfy the $\int_{(x,y)\in(X_a \times Y_b)} p\,(x^a, y^b|\lambda) = 1$.
3. The values observed by observers A and B are functions of the measurement settings (local detector) and the hidden parameter only: $x^a \equiv x(a, \lambda)$ and $y^b \equiv y(b, \lambda)$. That means that the experiment outcome variables x and y are conditional independent given the hidden state λ, and thus the Bell's "Factorizability" condition holds. We remind that the Factorizability (F) condition states the following:

   For any a, b, λ, there exist probability functions $p_1(x^a|\lambda)$ and $p_2(y^b|\lambda)$, such that $p\,(x^a, y^b|\lambda) = p_1(x^a|\lambda)\, p_2(y^b|\lambda)$. (F)

Now we can proceed by defining the marginal probabilities:

$$p_1(x^a|\lambda) \equiv \int_{Y_b} p\,(x^a, y^b|\lambda)\, dy \quad (1.3.1a)$$

$$p_2(y^b|\lambda) \equiv \int_{X_a} p\,(x^a, y^b|\lambda)\, dx^a \quad (1.3.1b)$$

Also we define as $A_\lambda(a, b)$ and $B_\lambda(a, b)$ the expectation values, for the hidden value λ, of the outcomes of experiments on system 1 and 2, respectively, when the settings are a, b. That is:

$$A_\lambda(a, b) \equiv \int_{X_a} x^a\, p_1(x^a|\lambda)\, dx^a \quad (1.3.2a)$$

$$B_\lambda(a,b) \equiv \int_{Y_b} y^b \, p_2(y^b|\lambda) \, dy^b \tag{1.3.2b}$$

We also define the expectation value of the product $x^a y^b$ of outcomes:

$$E_\lambda(a,b) \equiv \iint_{X_a \times Y_b} x^a y^b \; p\,(x^a, y^b|\lambda) \, dx^a dy^b \tag{1.3.3}$$

Note that all the expectation values above are functions of the hidden parameter λ and the experiment settings a, b.

Also, one can easily see that if the Factorizability condition (F) is satisfied, then the following is also true:

$$E_\lambda(a,b) = A_\lambda(a) \, B_\lambda(b) \tag{1.3.4a}$$

For simplicity, we will denote the expectation values $A_\lambda(a)$ and $B_\lambda(b)$ as $A(a,\lambda)$ and $B(b,\lambda)$ respectively. Therefore the previous relation becomes:

$$E_\lambda(a,b) = A(a,\lambda) \, B(b,\lambda) \tag{1.3.4b}$$

For the purpose of deriving the inequality we will use the special case of two possible experimental outcomes, that is $X_a = Y_b = \{\pm 1\}$, the same that Bell originally used.

Now consider the quantities:

$$S_\lambda(a,a',b,b') = |E_\lambda(a,b) + E_\lambda(a,b')| + |E_\lambda(a',b) - E_\lambda(a',b')| \tag{1.3.5}$$

We will define the expectation values of the E_λ functions with respect to the preparation distribution ρ of complete state λ:

$$C_\rho(a,b) \equiv \int_\Lambda E_\lambda(a,b) \, \rho(\lambda) \, d\lambda = \int_\Lambda A(a,\lambda) \, B(b,\lambda) \, \rho(\lambda) \, d\lambda \tag{1.3.6a}$$

$$C_\rho(a',b) \equiv \int_\Lambda E_\lambda(a',b) \, \rho(\lambda) \, d\lambda = \int_\Lambda A(a',\lambda) \, B(b,\lambda) \, \rho(\lambda) \, d\lambda \tag{1.3.6b}$$

$$C_\rho(a,b') \equiv \int_\Lambda E_\lambda(a,b') \, \rho(\lambda) \, d\lambda = \int_\Lambda A(a,\lambda) \, B(b',\lambda) \, \rho(\lambda) \, d\lambda \tag{1.3.6c}$$

$$C_\rho(a',b') \equiv \int_\Lambda E_\lambda(a',b') \, \rho(\lambda) \, d\lambda = \int_\Lambda A(a',\lambda) \, B(b',\lambda) \, \rho(\lambda) \, d\lambda \tag{1.3.6d}$$

The $C_\rho(a,b)$ denote the theoretical correlation of the two systems predicted by any HV theory, and in the special case of a bivalent experiment, such as Bell's, simply shows the expected value of a variable that indicates if the experimental outcomes of the two systems with the given settings a, b agree or not respectively.

Let S_ρ denote the corresponding relation between the expectation values C:

$$S_\rho(a,a',b,b') = \left|C_\rho(a,b) + C_\rho(a,b')\right| + \left|C_\rho(a',b) - C_\rho(a',b')\right| \tag{1.3.7}$$

We will also define the expectation value of the $S_\lambda(a,a',b,b')$ with respect to λ as:

$$E\big(S_\lambda(a,a',b,b')\big) \equiv \int_\Lambda S_\lambda(a,a',b,b')\,\rho(\lambda)\,d\lambda \tag{1.3.8}$$

Since the absolute value of the average of any random variable cannot be greater than the average of its absolute value, is clear that:

$$S_\rho(a,a',b,b') \le E\big(S_\lambda(a,a',b,b')\big) \tag{1.3.9}$$

Now, we will prove the first part of the theorem that follows from the Factorizability condition:

$$\begin{aligned} &S_\lambda(a,a',b,b') = |E_\lambda(a,b) + E_\lambda(a,b')| + |E_\lambda(a',b) - E_\lambda(a',b')| = \\ &|A(a,\lambda)B(b,\lambda) + A(a,\lambda)B(b',\lambda)| + |A(a',\lambda)B(b,\lambda) - A(a',\lambda)B(b',\lambda)| = \\ &\big|A(a,\lambda)\big(B(b,\lambda) + B(b',\lambda)\big)\big| + \big|A(a',\lambda)\big(B(b,\lambda) - B(b',\lambda)\big)\big| = \\ &|A(a,\lambda)||B(b,\lambda) + B(b',\lambda)| + |A(a',\lambda)||B(b,\lambda) - B(b',\lambda)| \end{aligned} \tag{1.3.10}$$

Knowing that the quantities $A(a,\lambda)$ and $A(a',\lambda)$, lie in the interval $[-1,1]$, we can conclude that:

$$S_\lambda(a,a',b,b') \le |B(b,\lambda) + B(b',\lambda)| + |B(b,\lambda) - B(b',\lambda)| \tag{1.3.11}$$

It is easy to check that:

$$|B(b,\lambda) + B(b',\lambda)| + |B(b,\lambda) - B(b',\lambda)| \le 2\max_\Lambda(|B(b,\lambda)|, |B(b',\lambda)|) \tag{1.3.12}$$

Since $B(b,\lambda)$ and $B(b',\lambda)$ also lie in the interval $[-1,1]$ from (1.11) and (1.12) we conclude that:

$$\forall\lambda \in \Lambda, \qquad S_\lambda(a,a',b,b') \le 2 \tag{1.3.13}$$

Since this bound holds for every value of λ, it must also hold for the expectation value of S_λ:

$$E\big(S_\lambda(a,a',b,b')\big) \leq 2 \tag{1.3.14}$$

So, we conclude that the basic Bell inequality that any hidden variable model should satisfy is:

$$S_\rho(a,a',b,b') \leq 2 \tag{1.3.15}$$

Using the triangular inequality, we can also derive another inequality, namely the CHSH inequality (Clauser et al. 1969), which is mostly used in the experimental applications or the literature.

$$\begin{aligned} 2 \geq S_\rho(a,a',b,b') &= \left|C_\rho(a,b) + C_\rho(a,b')\right| + \left|C_\rho(a',b) - C_\rho(a',b')\right| \\ &\geq \left|C_\rho(a,b) + C_\rho(a,b') + C_\rho(a',b) - C_\rho(a',b')\right| \end{aligned}$$

Summarizing, if a HV model describing the interactions between two bivalent systems, the correlations must satisfy the CHSH inequality:

$$2 \geq \left|C_\rho(a,b) + C_\rho(a,b') + C_\rho(a',b) - C_\rho(a',b')\right| \tag{1.3.16}$$

The final step of proving the Bell-type theorem is to exhibit a quantum mechanical system and a set of quantities for which the statistical predictions violate the CHSH inequality. Consider a pair of spin-½ particles that is produced in the following pure state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|1\rangle_1 \otimes |-1\rangle_2 - \frac{1}{\sqrt{2}}|-1\rangle_1 \otimes |1\rangle_2 \tag{1.3.17a}$$

Where $|1\rangle$ and $|-1\rangle$ are denoting the spin-up and spin-down eigenstates of spin respectively. The measurement of spin is performed on an arbitrary direction $\vec{n}$. We can write the state of the system simply as:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|1-1\rangle - \frac{1}{\sqrt{2}}|-11\rangle \tag{1.3.17b}$$

We can perform different spin measurements (Stern-Gerlach experiments) on this paired system with different directions. Each measurement is performed with respect to an axis which indicates the orientation of the measuring device, and can always has one of two possible outcomes: spin-up labeled with +1 and spin-down labeled with -1. If the experiments are done with the axes of the two devices aligned, the results are going to be always opposite. If the axes are perpendicular, the results are going to be probabilistically independent. In the general case, the directions of the measurements are given by two unit vectors $\vec{a}$ and $\vec{b}$, which in our case constitutes the experimental settings.

$$\vec{a} = (\sin\theta_a \cos\varphi_\alpha , \sin\theta_a \sin\varphi_\alpha , \cos\theta_a) \tag{1.3.18a}$$

$$\vec{b} = (\sin\theta_b \cos\varphi_b , \sin\theta_b \sin\varphi_b , \cos\theta_b) \tag{1.3.18b}$$

The spin operator of a bivalent system along an arbitrary direction $\vec{r}$, is according to quantum theory:

$$\boldsymbol{\sigma}_r = \begin{pmatrix} \cos\theta & \sin\theta\, e^{-i\varphi} \\ \sin\theta\, e^{i\varphi} & -\cos\theta \end{pmatrix}, \text{ where } \vec{r} = (\sin\theta\cos\varphi , \sin\theta\sin\varphi , \cos\theta) \tag{1.3.19}$$

Then, the expectation value of the product of the outcomes is given by

$$E_\psi(\vec{a},\vec{b}) = \langle\psi|\sigma_a^1 \otimes \sigma_b^2|\psi\rangle = -\cos\theta_a\cos\theta_b - \cos(\varphi_\alpha - \varphi_b)\sin\theta_a\sin\theta_b \tag{1.3.20}$$

Let us now take the vectors $\vec{n}$, $\vec{a}$ and $\vec{b}$ to be coplanar, and thus let, without the loss of generality, $\varphi_\alpha = \varphi_b$. Then the expectation value take the form

$$E_\psi(\vec{a},\vec{b}) = -\cos\theta_{ab}, \tag{1.3.21}$$

where $\theta_{ab} = \theta_a - \theta_b$ is the angle between vectors $\vec{a}$ and $\vec{b}$.

We choose four coplanar unit vectors $\vec{a}, \overrightarrow{a'}, \vec{b}, \overrightarrow{b'}$ such that $\theta_{ab} = \theta_{ab'} = \theta_{a'b} = \phi$ and therefore $\theta_{a'b'} = 3\phi$. Then, we are plugging the respective expected values into the expression for S. This choice yields:

$$\begin{aligned} S_\psi &= \left|E_\psi(\vec{a},\vec{b}) + E_\psi\left(\vec{a},\overrightarrow{b'}\right) + E_\psi\left(\overrightarrow{a'},\vec{b}\right) - E_\psi\left(\overrightarrow{a'},\overrightarrow{b'}\right)\right| \\ &= |\cos\theta_{ab} + \cos\theta_{ab'} + \cos\theta_{a'b} - \cos\theta_{a'b'}| \\ &= |3\cos\phi - \cos 3\phi| \end{aligned} \tag{1.3.22}$$

If we choose the angle ϕ accordingly, the expression (22) exceeds the CHSH bound, with maximum violation at $= \pm\frac{\pi}{4}$. For these angles we have:

$$S_\psi\left(\frac{\pi}{4}\right) = 2\sqrt{2} > 2 \tag{1.3.23}$$

That means, that if the Copenhagen interpretation is correct, an actual experiment on a pair of ½-spin systems would provide experimental evidence for disproving the hidden variable theory. The definite answer to that question came in 2015 (Hensen et al. 2015) when the experimental confirmation of Bell's theorem was conducted without any logical loopholes.

2 Contextuality

2.1 What is Quantum Contextuality?

As we have stated before, a big question that has concerned many scientists is whether or not we have the ability to assume the existence of objects and their properties, even when they have not been measured. This question started to have an actual meaning with the formulation of quantum mechanics and the phenomena that quantum theory describes. As we saw in previous sections, many scientists considered that the probabilistic nature of quantum mechanics was due to the theory's incompleteness, and thus the idea of a deterministic hidden variable theory governing the quantum world became more attractive. The explicit premise of the Hidden variables model is the principle of *Value definiteness* (VD) [Stanford Encyclopedia of Philosophy]:

(VD) *All observables defined for a Quantum Mechanical system have definite values at all times.*

Value definiteness is motivated from the assumption that the experiments are revealing values that exist independently of being measured. That suggests, a seemingly innocuous assumption, that of *non-contextuality* (NC) [Stanford Encyclopedia of Philosophy]:

(NC) *If a Quantum Mechanical system possesses a property (value of an observable), then it does so independently of any measurement context, i.e. independently of how that value is eventually measured.*

In 1964 Bell showed that there are cases of paired quantum systems, where a hidden variable model could never predict the systems behavior. After that, Kochen and Specker [Kochen-Specker 1967] proved a theorem that establishes a contradiction between (VD) and (NC), given that there is a 1-1 correspondence between properties of a quantum system and projection operators on the system's associated Hilbert space. That feature of quantum mechanics, i.e., the fact that measurements of quantum observables cannot simply be thought as revealing pre-existing values, is known as *Quantum Contextuality* (QC). More generally, contextuality refers as 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 state variables. Contextuality arises when a theory such as quantum mechanics, cannot be described by a joint probability distribution over a single probability space. That indicates the existence of experimental scenarios of that theory, where the statistics of observables cannot be described by a common joint probability distribution. However, there are subsets of the observable space, where the observables are indeed jointly measurable (commeasurable), and thus, a joint distribution can be constructed for that subset. From now on, we shall refer to such a set of commeasurable observables as observables that correspond to the same measuring *context*. One, may see the measuring context of a complete set of binary questions, whose answers are related to whether or not the post-measuring state lies in a specific subspace of the system's associated Hilbert space. More formally we can define the notion of *quantum measurement context* as follows:

2.1.1 Definition (Gudder, 2019)

A quantum measuring context, is a complete set of one-dimensional projections onto the subspaces of the system's associated Hilbert space. These subspaces are generated by pairwise orthogonal unit vectors. By complete set we mean that the set of these subspaces constitutes an orthogonal decomposition of the system's associated Hilbert space.

In other words, one might say that a theory is contextual, when a joint probability distribution that reproduces statistics of some contexts, cannot reproduce statistics of others at the same time [Grudka et al 2014].

It seems that contextuality, is a generic property of the logic that describes quantum theory. In fact, Bell's non-locality may be viewed as a special case of the more general phenomenon of contextuality, in which measurement contexts contain measurements that are distributed over space-like separated regions. This follows from the Fine-Abramsky-Brandenburger theorem that we is mentioned below.

Contextuality frameworks

Since its first demonstration by Bell-Kochen-Specker, the study of contextuality has developed into a major topic of interest, which led to the formulation of a number of more powerful mathematical frameworks, that were aim to generalize and study the concept of contextuality. The most important frameworks for contextuality are the following:

Contextuality-by-default framework

Contextuality-by-default consists a more natural way for someone to perceive the concept of contextuality. This framework utilizes probability theory and more specifically the theory of random variables [Dzhafarov et al 2016]. The Contextuality-by-default framework relates the "measurement contexts" with the "random variable contents", showing that contextuality is not just a feature of quantum theory, but a more general theory that can be applied and related to many different phenomena.

Sheaf-theoretic framework

Sheaf theory is primary concerned with the study of cohomology theories of general topological spaces with "general coefficient systems", providing a common method of defining and comparing different cohomology theories [Brendon 1997]. The sheaf-theoretic approach to contextuality [Abramsky-Brandenburger 2011] is a general mathematic setting, completely independent of the notion of Hilbert space, which strengthens the concept of Bell's non-locality and Kochen-Specker's quantum contextuality, and allows results to be proved in considerable generality. Thus, the sheaf-theoretic contextuality can be applied beyond quantum theory to any situation in which empirical data arises in contexts. In essence, contextuality arises when empirical data is *locally consistent* but *globally inconsistent*. This framework, also gives rise in a natural way to a qualitative hierarchy of contextuality:

Probabilistic Contextuality < Possibilistic Contextuality < Strong Contextuality

These three properties form a strict hierarchy, with the stronger one to imply the weaker ones, but not vice versa. For instance, Bell non-locality [Bell 1964], is weaker than Hardy non-locality (Hardy 1993), which is weaker than GHZ model [Greenburger et al 1990]. Abramsky and Brandenburger showed that the Kochen-Specker theorem is a strong contextuality theorem, and they provide a connection to graph theory defining the K-S contextuality in purely graph theoretic terms.

An interesting result of this theory, is the realization that the Factorizability condition of a hidden variable model, is a general property which subsumes both Bell-locality and a form of non-contextuality at the level of distributions as special cases. This means that the whole issue of non-locality and non-contextuality can be described in terms of obstructions to the existence of certain global sections. Another interesting point of the theory, is that the property of compatibility corresponds to a form of a generalized no-signaling principle, which the quantum theory of course satisfies.

As we have stated before, Arthur Fine showed that in a scenario where the CHSH inequality holds, a factorizable hidden variable model exists if and only if a noncontextual hidden variable model exists, in the sense of the existence of a joint distribution for the observables outcomes [Fine 1982]. This equivalence was proven to hold more generally in any experimental scenario by Abramsky and Brandenburger. For this reason, the fact that we can consider nonlocality as a special case of contextuality may be referred to as Fine-Abramsky-Brandenburger theorem (FAB):

(FAB) *Non-locality is a special case of contextuality.*

Operational framework

An extended notion of contextuality can also be applied to preparations and transformations as well as to measurements, within a general framework of operational physical theories [Spekkens 2005]. The term of operational physical theory, refers to a theory that describes the set of possible experiments that can be done with physical devices, and gives predictions about the probabilities of the outcomes in these experiments [Chiribella 2010]. With respect to measurements, this framework, removes the assumption of determinism of value assignments that is present in the standard definitions of contextuality. However, this breaks the interpretation of nonlocality as a special case of contextuality, and does not treat irreducible randomness as non-classical. In this framework the detection of non-locality is equivalent to the detection of contextuality, something that comes in opposition to the other contextuality frameworks. One way to partially resolve this issue, is to distinguish two shorts of locality according to the theory [Howard 1985]: Separability and local causality. A failure of local causality within the framework of a separable model does indeed imply a measurement of contextuality.

Graph-Theoretical framework

Another way to study the contextuality of different physical theories, is via Graph theory [Cabello et al 2014]. Within this framework experimental scenarios are described by graphs, and certain invariants of these graphs were shown to have a particular physical significance. The two basic graph types that this theoretical framework utilized, are the *compatibility graphs* and the *exclusivity graphs*. A compatibility or an exclusivity graph is a graph associated to a physical's system experimental scenario in the following way: The vertices in both graph types represent some of the system's observables that we are currently interested in. The edges of a compatibility graph represent the existence of a compatibility relation between the connected observables, i.e. they are jointly measurable. On the other hand, the edges of an exclusivity graph represent exclusivity relations, i.e. relations that satisfy the principle of consistent exclusivity (Cabello 2012). The principle of consistent exclusivity states that the sum of probabilities of pairwise exclusive events cannot exceed 1. The study of quantum contextuality can be conducted via the assignment of a truth value to each observable-vertex of a graph associated to a specific system. Contextuality may be witnessed in measurement statistics through the violation of non-contextuality inequalities.

Hypergraph framework

The Hypergraph theory provides a more refined way to describe the concept of contextuality than the graph-theoretical one [Acín et al 2015]. Although the basic idea is the same as in the graph theoretical approach, in this framework, the compatibility relations between observables are described via hyperedges, providing a more complete picture of the contextual nature of a theory's compatibility relations.

Quantifying Contextuality

There are many ways to quantify and measure contextuality. One approach is to measure "how much" a non-contextuality inequality is violated. Some known inequality examples are the KCBS inequality [Klyachko et al 2008] that we will analyze later, the Yu-Oh inequality [Yu-Oh 2011], or a Bell-type inequality [Bell 1964]. Another and more general way to measure contextuality is the *contextuality fraction* [Abramsky et al 2017]. For instructive reasons we will now present a short description about what contextuality fraction is.

First of all, we should clarify some notions. We will call *measuring scenario* an abstract description of a particular experimental setup, which consists of the triple $(X, \mathcal{M}, O)$ where: X is a set of finite measurements, O is a finite set of outcome values for each measurement, and $\mathcal{M}$ is a set of subsets of X. Each $C \in \mathcal{M}$ is called a *measurement context*, and represents a set of compatible measurements, i.e. a set of measurements that can be performed together. For each measurement context C, there is a probability distribution e_C on the joint outcomes of performing all the measurements in C; that is, on the set O^C of functions assigning an outcome in O to each measurement in C [Abramsky et al 2017].

Given two empirical models e and e' on the same measurement scenario, and $\lambda \in [0,1]$, one can define the empirical model $\lambda e + (1-\lambda)e'$ by taking the convex sum of probability distributions at each context. Compatibility is preserved by this convex sum, hence it yields a well-defined empirical model. Abramsky, Barbosa and Mansfield, wondered what fraction of a given empirical model e admits a non-contextual explanation. By using the empirical model which defined above, they ended up with a decomposition of each.

Let us consider a set of measurement statistics e, consisting of a probability distribution over joint outcomes for each measurement context. Based on the previous empirical model, we may factor the measurement model e into a non-contextual part e^{NC} and some remainder e', according to the following decomposition:

$$e = \lambda e^{NC} + (1-\lambda)e'$$

The maximum value of λ over all such decompositions is the noncontextual fraction of e denoted $NCF(e)$, while the remainder $CF(e) = 1 - NCF(e)$ is the contextual fraction of e. The basic idea behind that definition is that we look for a non-contextual explanation for the highest possible fraction of the data, and what is left over is the irreducibly contextual part. Indeed, for any such decomposition that maximizes λ, the leftover e' is proven to be strongly contextual. This measure of contextuality takes values in the interval $[0,1]$, where 0 corresponds to non-contextuality, and 1 corresponds to strong contextuality.

Finally, we should also mention that Quantum Contextuality has been identified as a source of quantum computational speedups and quantum advantage in quantum computing [Howard et al 2014].

2.2 Compatible observables

In order to study contextuality, we first need to understand what are the compatible observables and what the act of measuring two compatible observables implies. While in classical theories, the succession of the observables we measure does not have any impact on the results we obtain, in Quantum theory this is not the case. In many scenarios, measuring observables in different succession would provide us with different results. Consider for example the case where we perform measurements of two observables A and B on a system, with the following way: We first perform a measurement of the observable A, then of the observable B, and finally we measure the observable A once more. In a classical theory, one would expect that the outcomes of the measurements of A prior and after the measurement of B to be the same. However in quantum mechanics that is not always true. There are quantum observables whose order of measurement does not play any role on the results, and there are others that gives us different results depending on the order we measure them. We will call the ability to measure two or more observables simultaneously, and therefore in any order, commeasurability or compatibility, and the corresponding observables compatible. The ability to jointly measure a set of observables, implies the ability to construct a joint probability distribution for the measurement outcomes. The fact that we can construct a joint probability distribution over a set of mutually compatible observables is of great importance as we shall see in the process.

More formally, we shall say that the observables A_i, $i \in I$, are compatible if there exists an observable B and Borel functions f_i, $i \in I$, such that $A_i = f_i(B)$, $\forall\, i \in I$ (Kochen-Specker 1967). It is clear, that if this statement is true, one can measure simultaneously the observables A_i by measuring B and applying the function f_i to the measured value. In the case of quantum mechanics, the above definition coincides with the pairwise commutability of the observables' associated operators. This can be easily seen by applying the spectral decomposition theorem.

We may also define an algebra over a set of compatible observables as following: If A_1 and A_2 are compatible, is implied that $A_1 = f_1(B)$ and $A_2 = f_2(B)$. Then we can easily define the observables $(\mu_1 A_1 + \mu_2 A_2)$ and $A_1 A_2$ for all real μ_1, μ_2, as:

$$\mu_1 A_1 + \mu_2 A_2 = (\mu_1 f_1 + \mu_2 f_2)(B) \qquad (2.2.1)$$

$$A_1 A_2 = (f_1 f_2)(B) \qquad (2.2.2)$$

By defining the linear combinations and the products of compatible observables, the set of all observables acquires the structure of a partial algebra, which we will define later.

Having stated all the necessary notions for observables' compatibility, we are going to present a useful theorem about the quantum observables compatibility:

2.2.1 The Compatibility Theorem (Shankar, 1994)

Let us have two observables A and B, and their associated operators $\tilde{A}$ and $\tilde{B}$ respectively. Then the following statements are equivalent:

- A and B are compatible observables.
- $\tilde{A}$ and $\tilde{B}$ share a common eigenbasis.
- $\tilde{A}$ and $\tilde{B}$ commute, that is $[\tilde{A}, \tilde{B}] = 0$.

This is a very useful theorem, especially in the cases of finite dimensional quantum systems that we are going to study in the next sections.

2.3 Kochen & Specker Theorem

After the efforts of John Bell to construct an inequality that identifies the existence of non-local correlations, it became clear that quantum mechanics is not compatible with a hidden variable theory. Kochen and Specker, believed that the notion of Bell's non-locality is not limited on the spatial separated multipartite systems, and that constitutes a more fundamental property of Quantum mechanics which can be extended to the measurements of every quantum system. Gleason has already proved in 1957 that the assignment of probabilities on the measurement outcomes is independent of the measurement context [Gleason 1957]. This theorem provided a new baseline for the interpretation of Quantum mechanics, since the aforementioned property, known as Gleason's property, underlies all the Quantum theoretical scenarios. Kochen and Specker initially assumed the existence of a hidden variable model that allows the joint measurement of all the involved observables of an at least three-dimensional arbitrary quantum system. Then they showed that this assumption leads to contradictions.

Hidden Variable Model

However, a natural question that arises is what do we mean by asking whether this quantum description can be embedded into a classical theory, or be replaced by a theory of hidden variables?

First, let describe the basic framework of a physical theory. Let $\mathcal{O}$ be the set of the theory's observables, i.e. the physical quantities we are measure, and $\mathcal{S}$ be the set of the system's possible states. Additionally, we have a function P that assigns to each observable A and each state ψ a probability measure P_ψ^A, with which we can calculate the expectation value of the observable A for the state ψ in the usual manner:

$$Exp_\psi(A) = \int_{-\infty}^{\infty} \lambda \, dP_\psi^A(\lambda) \tag{2.3.1}$$

States are generally divided into pure and mixed states. Roughly speaking, the pure states describe a maximal possible amount of knowledge about the physical system in question, while the mixed states give only incomplete information and describe our ignorance of the exact pure state the system is actually in. In a classical theory, given that ψ is a pure state, the probability P_{ψ}^{A} assigned to each observable is an atomic measure concentrated on a real number α. That is, $P_{\psi}^{A}(U) = 1$ if $\alpha \in U$ and $P_{\psi}^{A}(U) = 0$ if $\alpha \notin U$. Therefore, we can introduce the phase space Ω of pure states, where each observable A becomes associated with a real valued function $f_A : \Omega \to \mathbb{R}$ given by $f_A(\psi) = \alpha$.

In the case of a well-defined Quantum mechanical system, the set of observables $\mathcal{O}$ is represented by a set of self-adjoint operators of a Hilbert space $\mathcal{H}$, while the set of pure states $\mathcal{S}$ is the set of all the unit Hilbert rays. For each observable $A \in \mathcal{O}$ we denote by $E^A(\cdot)$ (projection valued) the spectral measure of A, and we have the spectral decomposition:

$$A = \int_{\sigma(A)} \lambda \, dE^A(\lambda) \tag{2.3.2}$$

Where $\sigma(A)$ denotes the spectrum of A. More generally, the operator $u(A)$ for a Borel function $u : \mathbb{R} \longrightarrow \mathbb{R}$ has the representation:

$$u(A) = \int_{\sigma(A)} u(\lambda) \, dE^A(\lambda) \tag{2.3.3}$$

Then we have that

$$P_{\psi}^{A}(U) = \langle E^A(U)\psi, \psi \rangle \tag{2.3.4}$$

Where ψ is any unit vector in the one-dimensional linear subspace corresponding to the pure state $|\psi\rangle$. Hence, by the spectral theorem we obtain

$$Exp_{\psi}(A) = \langle A \rangle_{\psi} = \int_{\sigma(A)} \lambda \, d\langle E^A(U)\psi, \psi \rangle = \langle A\psi, \psi \rangle \tag{2.3.5}$$

Therefore, the minimal requirement for the existence of a Hidden Variable model, is that there should exist a measurable space $(\Omega, \mathcal{F})$, where $\mathcal{F}$ denotes the σ-algebra of measurable subsets of Ω, and two maps

$$\mathcal{O} \ni A \longmapsto f_A : \Omega \longrightarrow \mathbb{R} \text{ , measurable} \tag{2.3.6}$$

$$\mathcal{S} \ni |\psi\rangle \longmapsto \mu_{\psi} : \text{probability measure on } (\Omega, \mathcal{F}) \tag{2.3.7}$$

such that the probability distributions are reproduced:

(KS1) $$P_\psi^A(U) = \mu_\psi\big(f_A^{-1}(U)\big) \tag{2.3.8}$$

The first map assigns "values" to each observable. The second one, assigns a probability measure to every pure state, such that the value of $P_{|\psi\rangle}^A(U)$ expresses the probability the outcome of measuring observable A for a system in the state $|\psi\rangle$, to lie inside the measurable real subset U. In particular, the expectation values have to agree:

$$\langle A\rangle_\psi = \langle\psi, A\psi\rangle = \int_{\sigma(A)} \lambda\, dP_\psi^A(\lambda) = \int_\Omega f_A(\omega) d\mu_\psi(\omega) \tag{2.3.9}$$

As long as not more is required, we can introduce a hidden variable model which is quite "natural" from probability theory's perspective. Kochen and Specker provided us with that model via the mathematical construction of a phase space Ω for which (2.3.6) and (2.3.7) are satisfied:

$$\Omega = \mathbb{R}^{\mathcal{O}} = \{\omega | \omega : \mathcal{O} \longrightarrow \mathbb{R}\},\ \mathcal{F} = \mathcal{B}^{\mathcal{O}} \tag{2.3.10}$$

Where $\mathcal{B}$ is a σ-algebra of $\mathbb{R}$, and the two maps f_A and $\mu_{|\psi\rangle}$ are given by

$f_A(\omega) = \omega(A)$, canonical projection

$\mu_\psi = \prod_{A\in\mathcal{O}} P_\psi^A$, product measure

Then (KS1) is indeed satisfied

$$\mu_\psi\big(f_A^{-1}(U)\big) = \mu_\psi(\{\omega | f_A(\omega) \in U\}) = \mu_\psi(\{\omega | \omega(A) \in U\}) = P_\psi^A(U) \tag{2.3.11}$$

Note that in the construction of this phase space, we consider the functions f_A to be measurable with respect to the probability measure μ_ψ. Thus, according to probability theory these observables can be interpreted as random variables for each state $|\psi\rangle$. Furthermore, it is easily understood that in this representation the observables appear as independent random variables. However, the observables of a physical theory are not always independent, and therefore we have to add some additional condition, in order to adapt this mathematical construct to a physically interesting theory.

2.3.1 Definition (Kochen-Specker 1967)

We define the observable $g(A)$ for every observable A and a measurable function $g : \mathbb{R} \longrightarrow \mathbb{R}$ by the formula

$$P_\psi^{g(A)}(U) = P_\psi^A\big(g^{-1}(U)\big), \qquad \forall\psi \in \mathcal{S} \tag{2.3.12}$$

If we assume that every observable is determined by the function P, i.e. $P_\psi^A = P_\psi^B,\ \forall \psi \in \mathcal{S} \Longrightarrow A = B$, then the formula (2.3.12) defines the observable $g(A)$. This definition coincides with the definition of a function of an observable in both quantum and classical mechanics.

Notice that the measurement of $g(A)$ is independent of the theory considered, as one can consider the value $g(a)$ as a measurement outcome of the observable $g(A)$, if the measured value of observable A is a. Thus, the set of observables acquires an algebraic structure, and the introduction of hidden variables should preserve this structure. Therefore it is very natural to require that a hidden variable model should also satisfy

(KS2) $$f_{g(A)} = g(f_A) \tag{2.3.13}$$

for every measurable function $g : \mathbb{R} \longrightarrow \mathbb{R}$ and every observable $A \in \mathcal{O}$.

This second condition has far reaching consequences. It should be regarded as an alternatively to Bell's locality assumption (Straumann 2018).

The following remark will be important.

2.3.2 Remark (Straumann 2018)

If $A_1, A_2 \in \mathcal{O}$ are two *commuting* observables then the following are true

$$f_{A_1 A_2} = f_{A_1} \cdot f_{A_2} \tag{2.3.14}$$

$$f_{A_1 + A_2} = f_{A_1} + f_{A_2} \tag{2.3.15}$$

Proof:

Since the A_1, A_2 are commuting self-adjoint operators we know from a theorem [von Neumann 1955] that they can represented as real measurable functions of a single self-adjoint operator B:

$$A_1 = u_1(B)\ ,\ A_2 = u_2(B)\ , \text{ where } u_1, u_2 \text{ are measurable real functions}$$

Then we have that:

$$A_1\, A_2 = u_1(B)\, u_2(B) = (u_1 \cdot u_2)(B)$$

Thus, for the product we have

$$f_{A_1 A_2} = f_{(u_1 \cdot u_2)(B)} = (u_1 \cdot u_2) \circ f_B = (u_1 \circ f_B) \cdot (u_2 \circ f_B)$$
$$= f_{u_1(B)} \cdot f_{u_2(B)} = f_{A_1} \cdot f_{A_2}$$

The additivity follows similarly.

Note that in Bell's work, the product rule or Factorizability condition follows for separated situations from his locality assumption, however not only for compatible observables.

The algebraic structure of the Compatibility relation

The pure states of a quantum system can be represented by one dimensional linear subspaces of a Hilbert space whose dimension is given by the number of possible outcomes we can observe. On the other hand, the observables are represented by Hermitian operators on that space, and all the observed outcomes upon measurement are the eigenvalues of the observable's associated operator. The pre-measuring state determines the probability that each outcome occurs, and the post-measuring state always lie on the corresponding eigenspace of the eigenvalue that we measured. Additionally, we know that when two observables are compatible, their associated operators commute, and that the set of commuting operators is not transitive. Therefore, if we want to study the logic that underlies the quantum measurement outcomes, we need to study the logic of Hilbert space's linear subspaces, and the properties of the operator's compatibility relation.

In their original paper, Kochen and Specker [Kochen-Specker, 1967] in order to describe a logical procedure for assigning truth values to the measurement outcomes of the observables, they devised the notion of a *partial algebra*. A partial algebra is basically the algebraic structure that describes the set of observables of a quantum system.

2.3.3 Definition (Kochen-Specker 1967)

A set A forms a *partial algebra over a field* K if there is a binary relation of *Compatibility* on $\odot \subseteq A \times A$, the operations of addition $+ : \odot \longrightarrow A$ and multiplication $* : \odot \longrightarrow A$, a scalar multiplication $\cdot : K \times A \longrightarrow A$, and an element $1 \in A$, satisfying the following properties:

1. The relation $\odot$ is reflexive and symmetric, i.e. $a \odot a$, and $a \odot b \Longrightarrow b \odot a$, $\forall a, b \in A$.
2. $a \odot 1$, $\forall a \in A$.
3. The relation $\odot$ is closed under the operations, i.e. If $a_i \odot a_j$, $\forall\, 1 \leq i, j \leq 3 \Longrightarrow (a_1 + a_2) \odot a_3$, $(a_1 a_2) \odot a_3$ and $\lambda a_1 \odot a_3$, $\forall \lambda \in K$.
4. If $a_i \odot a_j$, $\forall\, 1 \leq i, j \leq 3$, then the values of the polynomials in a_1, a_2, a_3 form a commutative algebra over the field K.

Of special interest are the cases in which the field K is the field of real numbers $\mathbb{R}$, and the field of two elements $\mathbb{Z}_2$. For the case of a partial algebra over $\mathbb{Z}_2$ we may define the Boolean operations in terms of the ring operations in the usual manner: $a' = 1 - a$, $a \wedge b = ab$, $a \vee b = a + b - ab$. It follows that if $a_i \circledcirc a_j$, $\forall\ 1 \leq i, j \leq 3$, then the polynomials in a_1, a_2, a_3 form a *Boolean Algebra.*

2.3.4 Definition (Kochen-Specker 1967)

We shall call a partial algebra over $\mathbb{Z}_2$ a *partial Boolean algebra.*

What makes a partial Boolean algebra interesting, is the fact that the set of idempotent elements, i.e. the elements for which $a^2 = a$ is true, of a partial algebra $\mathfrak{P}$, forms a partial Boolean algebra. That is deduced from the familiar fact that the set of idempotents of a commutative algebra forms a Boolean algebra.

Now, let $\mathcal{H}_n$ be a complex Hilbert space of dimension of n, and $H(\mathcal{H}_n)$ be the set of all self-adjoint operators on $\mathcal{H}_n$. If we take the relation of compatibility to be the relation of commutativity then $H(\mathcal{H}_n)$ forms a partial algebra over $\mathbb{R}$. Thus the set $B(\mathcal{H}_n)$ of the orthogonal projections of $\mathcal{H}_n$ forms a partial Boolean algebra. Because every projection corresponds uniquely to a closed linear subspace of $\mathcal{H}_n$, we may alternatively consider $B(\mathcal{H}_n)$ as the partial Boolean algebra of the closed linear subspaces of $\mathcal{H}_n$, with the operation $a \wedge b$ to be the intersection of the subspaces a and b, and the operation $a \vee b$ to be the direct sum of these subspaces. That is:

$$a \wedge b = a \cap b$$

$$a \vee b = \overline{a \oplus b} \qquad (2.3.16)$$

a' denotes the orthogonal complement of a

Notice that since each observable is characterized from the eigenspaces of its associated Hermitian operator, the set $\mathcal{O}$ of observables of a physical theory forms a partial algebra over $\mathbb{R}$ due to the relation of compatibility. If observable P is a projector, or alternatively an idempotent element of $\mathcal{O}$, then it follows from the definition of P^2, that the measured values of the observable P can only be 1 or 0. By labelling these values as truth and falsity respectively, we may consider each such projection observable as a proposition of the theory (von Neumann 1955). Thus, the set of propositions of a physical theory forms a partial Boolean algebra. This implies that:

The propositions of quantum mechanics form a partial Boolean sub-algebra $\mathfrak{B}$ ***of*** $\boldsymbol{B(\mathcal{H}_n)}$ (Kochen-Specker 1967).

In order to compare structurally two partial algebras U, V we are going to define a *homomorphism* between them.

2.3.5 Definition (Kochen-Specker 1967)

A map $f: U \longrightarrow V$ between two partial algebras over a common field K is a *homomorphism* if for every $a, b \in U$ such that $a \odot b$ and for every $\mu, \lambda \in K$, the following are true:

1. $f(a) \odot f(b)$,
2. $f(\mu a + \lambda b) = \mu f(a) + \lambda f(b)$,
3. $f(ab) = f(a)f(b)$,
4. $f(1) = 1$.

It is obvious that we defined the homomorphism in such a way that the relation of compatibility is preserved.

The Hidden Variable model on Compatible Observables

As we stated above, the basic assumptions which Kochen and Specker made for a Hidden variable model can be summarized in the existence of a phase space where:

1. There is always a state distribution, and every observable A of the set of observables $\mathcal{O}$ is unambiguously mapped onto a real number such that:

   (KS1) $P_\psi^A(U) = \mu_\psi\left(f_A^{-1}(U)\right)$, where $U \subseteq \mathbb{R}$ measurable

2. Values of all observables in $\mathcal{O}$ conform to the following constraint:

   (KS2) $f_{g(A)} = g(f_A)$, for every measurable real function g.

Now let us see what a hidden variable model implies for the partial algebra of quantum observables. Consider the set $\mathbb{R}^\Omega$ of all function from the hidden space Ω into the $\mathbb{R}$, i.e. $\mathbb{R}^\Omega = \{f | f : \Omega \longrightarrow \mathbb{R}\}$. It is obvious that $\mathbb{R}^\Omega$ with the usual operations of function addition and multiplication, forms a commutative algebra over $\mathbb{R}$. From remark (2.3.2), it is clear that if anyone assumes a hidden variable model, then the partial algebra Q of quantum mechanical observables becomes a partial algebra of functions $f : \Omega \longrightarrow \mathbb{R}$ with the same partial function operations as in the case of $\mathbb{R}^{\Omega}$. That implies that there must be an injective homomorphism from the partial algebra Q into the commutative algebra $\mathbb{R}^{\Omega}$. The conclusion of Kochen and Specker was the following:

A necessary condition for the existence of hidden variables for quantum mechanics is the existence of an embedding of the partial algebra $\boldsymbol{Q}$ of quantum mechanical observables into a commutative algebra.

Now if $\varphi : \mathfrak{P} \hookrightarrow \mathcal{C}$ is an embedding of a partial algebra $\mathfrak{P}$ into a commutative algebra $\mathcal{C}$, it follows immediately that the restriction of φ onto the partial Boolean algebra of idempotent elements of $\mathfrak{P}$, is an embedding into the Boolean algebra of idempotent elements of $\mathcal{C}$. Thus, the existence of hidden variables implies the existence of an embedding of the partial Boolean algebra of quantum-mechanical propositions into a Boolean algebra.

If we assume the existence of a hidden state space Ω, so that the partial algebra of quantum mechanical observables Q is embeddable by a map f into the algebra $\mathbb{R}^{\Omega}$, then each hidden state $\omega \in \mathbb{R}^{\Omega}$ defines a homomorphism $h : Q \longrightarrow \mathbb{R}$ with $h(A) = f_A(\omega)$, which physically speaking may considered as a prediction function which simultaneously assigns a predicted measured value to every observable. Thus, the existence of hidden variables implies the existence of a large number of prediction functions. Every homomorphism from a partial to the real numbers, is by restriction a homomorphism of the partial Boolean algebra of idempotents onto $\mathbb{Z}_2$. The following theorem characterizes the embedding of a partial Boolean algebra into a Boolean algebra in terms of its homomorphisms onto $\mathbb{Z}_2$.

2.3.6 Theorem (Kochen-Specker 1967)

Let $\mathbb{B}$ be a partial Boolean algebra. A necessary and sufficient condition that $\mathbb{B}$ is embeddable in a Boolean algebra $\boldsymbol{B}$ is that for every pair of distinct elements $a, b \in \mathbb{B}$ there is a homomorphism $h : \mathbb{B} \to \mathbb{Z}_2$ such that $h(a) \neq h(b)$.

Proof:

($\Longrightarrow$) Suppose that $\varphi : \mathbb{B} \to \boldsymbol{B}$ is an embedding. Since $\varphi(a) \neq \varphi(b)$ if $a \neq b$, there exists by the semi-simplicity property of Boolean algebras [Halmos 1963], a homomorphism $g : \boldsymbol{B} \to \mathbb{Z}_2$ such that $(g \circ \varphi)(a) \neq (g \circ \varphi)(b)$. Hence $h = g \circ \varphi$ is the required homomorphism of $\mathbb{B}$ onto $\mathbb{Z}_2$.

($\Longleftarrow$) Let S be the set of all non-trivial homomorphisms of $\mathbb{B}$ onto $\mathbb{Z}_2$. Define the map $\varphi : \mathbb{B} \to \mathbb{Z}_2^S = \{f | f : S \to \mathbb{Z}_2\}$ by letting $\mathbb{B} \ni a \mapsto g : S \to \mathbb{Z}_2$ such that $g(h) = h(a)$, $\forall h \in S$. Then it easily checked that φ is an embedding of $\mathbb{B}$ into the Boolean algebra $\mathbb{Z}_2^S$.

□

The previous theorem essentially states that if a partial Boolean algebra is embeddable into a Boolean algebra, one can find a way to assign truth values "0" and "1" to every element of the partial Boolean algebra, such that two compatible elements could never take the "1" value simultaneously.

A useful way to visualize is via an orthogonality graph. An orthogonality graph is a graph of orthogonal relations on Hilbert space, meaning that every vertex represents a 1-dimensional Hilbert subspace, and every edge denotes the orthogonality relation between the connected vertices.

After the introduction of the basic framework, we can finally formulate the Kochen & Specker theorem.

Kochen Specker proof

K-S Theorem (Kochen-Specker 1967)

If $\boldsymbol{dim\mathcal{H}} > 2$*, an embedding, satisfying (KS1) and (KS2), is in general not possible.*

Let $\mathbb{B}(\mathcal{H})$ denote the partial Boolean algebra of the propositions of linear subspaces of $\mathcal{H}$. In order to prove the K-S theorem, we will consider an orthogonality graph of the rays belonging to the Hilbert space $\mathcal{H}$. In this graph, each vertex represents a Hilbert space's ray, and each edge denotes the orthogonal relation between the corresponding rays of the connected vertices. It is easy perceivable that this graph represents a finite Boolean sub-algebra of $\mathbb{B}(\mathcal{H})$. So, we are going to show that there is always a sub-algebra D of $\mathbb{B}(\mathcal{H})$, such that there is no homomorphism from D to $\mathbb{Z}_2$.

As it turns out the Kochen-Specker can be reduced to a "coloring type problem", meaning that if a hidden variable theory is the case, one can assign binary values to any orthogonality graph of a system with $\boldsymbol{dim\mathcal{H}} > 2$, in a way that every neighborhood of the graph has exactly one element with the value 1.

It is obvious that if such a graph, where an assignment of truth values is impossible, exists for a 3-dimensional Hilbert space, it also exists for higher dimensions, since the addition of extra edges in the graph, can only make our proof simpler.

2.3.7 Definition

We will say that a graph G is realizable on a finite dimensional Hilbert space $\mathcal{H}$, when G constitutes a graph of the rays' orthogonal relation on $\mathcal{H}$. That means, that there is an assignment of unit elements of $\mathcal{H}$ to the vertices of G, such that distinct elements are associated with distinct vertices, and the orthogonality relation between two elements is denoted by an edge connecting the corresponding vertices.

Therefore, in order to prove K-S theorem we shall show that there is a realizable graph on the 3-dimensional Euclidean space E^3, in which an assignment of binary values on the vertices that satisfy the above conditions is not possible.

For simplicity, we will consider that the points that the graph vertices represent lie unit sphere S.

2.3.8 Lemma

The following graph G_1 is realizable on S.

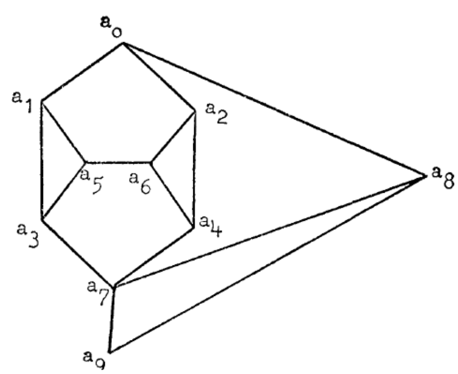


Fig. 2.3.1 Graph of orthogonal relations in R^3

In fact, it can be proven that if A_0 and A_9 are the corresponding unit vectors of the vertices a_0 and a_9 respectively, and the angle θ between those vectors is satisfying the relation $0 \leq \theta \leq \arcsin\left(\frac{1}{3}\right)$, then the graph G_1 is realizable on S.

Proof

Let $u : V(G_1) \to S$ be an injective map that maps each vertex a_i of the G_1 to a point $A_i = u(a_i)$ on the unit sphere S. Now, let us assume that θ, the angle between $u(a_0)$ and $u(a_9)$, is any acute angle. Since $u(a_8)$ is orthogonal to $u(a_0)$ and $u(a_9)$, and $u(a_7)$ is orthogonal to $u(a_8)$, $u(a_7)$ must lie in the plane defined by $u(a_0)$ and $u(a_9)$. Moreover, since the $u(a_7)$ is orthogonal to $u(a_9)$, we have that the angle φ between $u(a_7)$ and $u(a_0)$ is $\varphi = \frac{\pi}{2} \pm \theta$. Let us chose the $u(a_7)$ such that the central angle $\varphi = \frac{\pi}{2} - \theta$.

Now, let $u(a_5) = \vec{\imath}$ and $u(a_6) = \vec{k}$ and then choose another vector $\vec{\jmath}$ such that $\vec{\imath}, \vec{\jmath}, \vec{k}$ form a complete set of orthonormal vectors. Given that, the vector $u(a_1)$ being orthogonal to $\vec{\imath}$, may be written as:

$u(a_1) = \frac{1}{\sqrt{1+x^2}}\left(\vec{\jmath} + x\vec{k}\right)$, for a suitable $x \in \mathbb{R}$.

Similarly, $u(a_2)$ being orthogonal to $\vec{k}$, may be written as:

$u(a_2) = \frac{1}{\sqrt{1+y^2}}(\vec{\imath} + y\vec{\jmath})$, for a suitable $y \in \mathbb{R}$.

Then, the orthogonality relations of the graph yield:

$u(a_3) = u(a_5) \times u(a_1) = \frac{1}{\sqrt{1+x^2}}\left(-x\vec{\jmath} + \vec{k}\right)$,

$u(a_3) = u(a_5) \times u(a_1) = \frac{1}{\sqrt{1+y^2}}(y\vec{\imath} - \vec{\jmath})$,

Now, $u(a_0)$ is orthogonal to $u(a_1)$ and $u(a_2)$, so:

$$u(a_0) = \frac{u(a_1) \times u(a_2)}{\|u(a_1) \times u(a_2)\|} = \frac{1}{\sqrt{1 + x^2 + x^2y^2}}\left(-xy\vec{\imath} + x\vec{\jmath} - \vec{k}\right)$$

Similarly, $u(a_7)$ is orthogonal to $u(a_3)$ and $u(a_4)$, so:

$$u(a_7) = \frac{u(a_4) \times u(a_3)}{\|u(a_4) \times u(a_3)\|} = \frac{1}{\sqrt{1 + y^2 + x^2y^2}}\left(-\vec{\imath} - y\vec{\jmath} - xy\vec{k}\right)$$

Recalling now that the usual inner product of two unit vectors just equals the cosine of the angle between them, we get:

$$u(a_0)\, u(a_7) = \cos\varphi = \frac{xy}{\sqrt{(1 + x^2 + x^2y^2)(1 + y^2 + x^2y^2)}}$$

But since $\varphi = \frac{\pi}{2} - \theta$, we get that:

$$\sin\theta = \frac{xy}{\sqrt{(1 + x^2 + x^2y^2)(1 + y^2 + x^2y^2)}}$$

By using elementary calculus we can easily show that the previous expression achieves a maximum value of $1/3$ for $x = y = \pm 1$. Hence, the graph G_1 is realizable if $0 \le \sin\theta \le \frac{1}{3}$ or equivalently when $0 \le \theta \le \arcsin\left(\frac{1}{3}\right)$.

□

2.3.9 Lemma

The following graph G_2 is realizable on S.

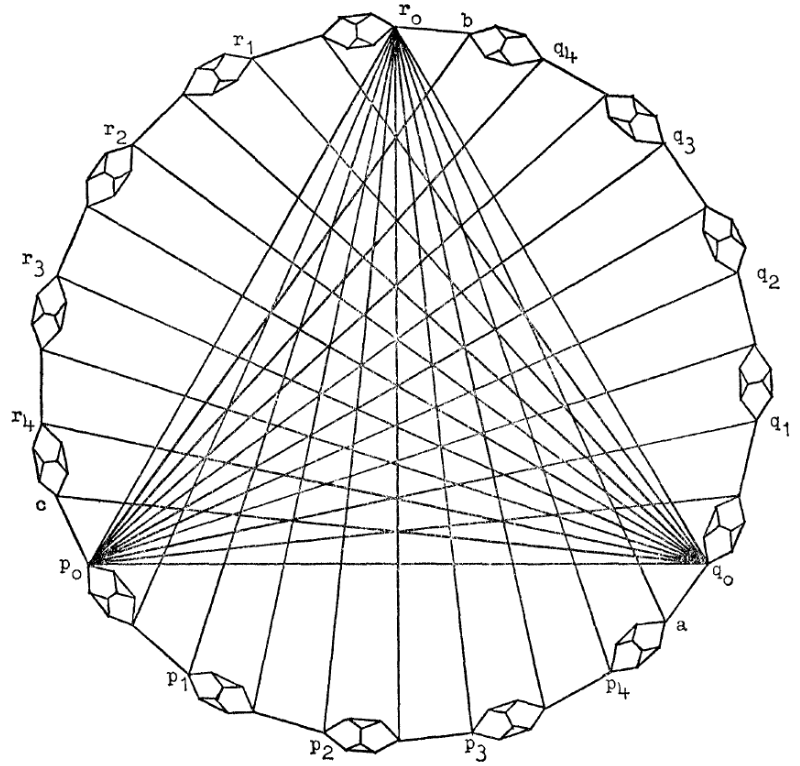


Fig. 2.3.2 Graph G_2 of orthogonal relations in $\mathbb{R}^3$, which is constructed with isomorphic copies of graph G_1

Proof:

The graph G_2 can be constructed by combining isomorphic copies of the graph G_1 in the following way: First consider a realization of graph G_1 for an angle of $18°$. Since $\theta = \frac{\pi}{10} < \arcsin\frac{1}{3} \cong 0.3398$ the graph G_1 is indeed realizable on the unit sphere S. Now, choose three orthogonal points P_0, Q_0, R_0 on the unit sphere and place interlocking copies of G_1 between every two of them, such that every instance of point a_9 of one copy, is identified with the instance of a_0 of the next copy. These copies of G_1, are placed between every two of the initial three orthogonal points P_0, Q_0, R_0, in a way that the movement from a specific instance of point a_i of one copy to the respective instance of point a_i of its immediate interlocking neighbor copy, is equivalent to a rotation by $18°$ about the axis that goes through the origin and the third of the initial orthogonal points. Due to the fact that P_0, Q_0, R_0 are orthogonal, we can fit five copies of G_1 between any two of them, since $\varphi_{P_0Q_0} = \varphi_{P_0R_0} = \varphi_{Q_0R_0} = \frac{\pi}{2} = 5\theta$. In this way, five interlocking copies of G_1 are spaced between, say, P_0 and Q_0 and all five instances of a_8 are identified with R_0. Also, anyone can see that the orthogonality between the points a_0 and a_9 of each copy that is placed between P_0 and Q_0, and R_0 is evidently conserved. Of course, similar results are yielded about the placement of interlocking copies of G_1 between $P_0 - R_0$ and $Q_0 - R_0$.

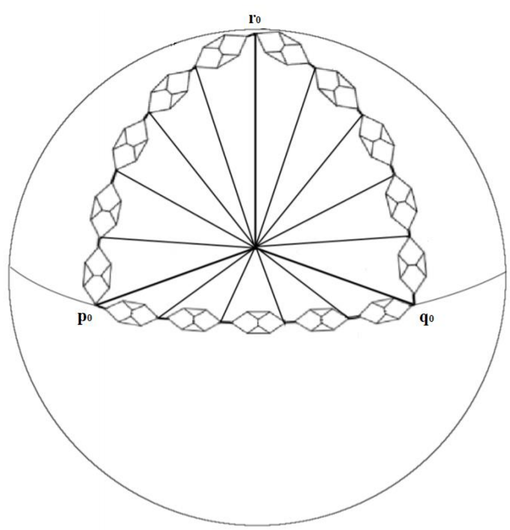


Fig. 2.3.3 A figure showing how 15 copies of G_1 are placed between three orthogonal points in the 3-dimensional unit sphere.

A more rigorous way to express the exact position of the point a_0 of every G_1-copy is by assuming an injective map $u : V(G_2) \to S$ that maps each vertex v_i of the G_2 to a point $V_i = u(v_i)$ on the unit sphere S. Let $u(p_k) = P_k$, $u(q_k) = Q_k$, $u(r_k) = R_k$, for $0 \leq k \leq 4$, be the corresponding unit vectors to the vertices of G_2, as shown in the diagram (Fig. 2.3.3).

Now, we can define the corresponding points of the vertices noted on the diagram above as following:

$$P_k = \cos\frac{k\pi}{10}\vec{\imath} + \sin\frac{k\pi}{10}\vec{\jmath}$$

$$Q_k = \cos\frac{k\pi}{10}\vec{\jmath} + \sin\frac{k\pi}{10}\vec{k}$$

$$R_k = \cos\frac{k\pi}{10}\vec{\imath} + \sin\frac{k\pi}{10}\vec{k}$$

where $0 \leq k \leq 4$, and $\vec{\imath}, \vec{\jmath}, \vec{k}$ be a complete set of orthonormal vectors on $\mathbb{R}^3$.

It is pretty obvious that the initial three orthogonal points P_0, Q_0, R_0 that we mentioned before correspond to the vertices p_0, q_0, r_0 respectively, according to the diagram.

□

As we have stated before, each graph of orthogonal relations on E^3 is associated with a partial Boolean sub-algebra $\mathbb{B}(E^3)$ of the linear subspaces of E^3. Let T be the image of G_2 under the injective map u, consisting of 117 points on S. Now, let D be the partial Boolean sub-algebra generated by T in $\mathbb{B}(E^3)$. This corresponds to completing the graph G_2 so that every edge lies in a triangle. In the resulting graph the points and edges correspond to one and two dimensional linear subspaces of $\mathbb{B}(E^3)$ respectively.

Now, consider a homomorphism $h : D \to \mathbb{Z}_2$, where D is a partial Boolean sub-algebra of $\mathbb{B}(E^3)$. If s_1, s_2, s_3 are three mutual orthogonal rays of D, then the following must be true:

$$\begin{aligned} &h(s_1) \cup h(s_2) \cup h(s_3) = h(s_1 \cup s_2 \cup s_3) = h(E^3) = 1 \text{ , and} \\ &h(s_i) \cup h(s_j) = h(s_i \cup s_j) = h(0) = 0 \text{ , } 1 \leq i \neq j \leq 3 \end{aligned} \tag{2.3.17}$$

Hence, exactly one of every three mutually orthogonal lines is mapped by h onto 1. Now we can finally prove the K-S theorem

2.3.10 Theorem

The finite partial Boolean algebra D has no homomorphism onto $\mathbb{Z}_2$

Proof

Let assume that such a homomorphism exists. As we have seen, such a homomorphism $h : D \to \mathbb{Z}_2$ induces a map $h^* : T \to \{0,1\}$ that satisfies the condition (2.3.17).

Therefore, we should assume that there is a map $g : G_2 \to \{0,1\}$ satisfying condition (2.3.17). That means that there is at least one way to "color" binary the vertices of G_2. Let us now, observe how this map g acts on a copy of G_1 as a subgraph of G_2. Suppose that $g(a_0) = 1$, then it follows that $g(a_9) = 1$. That happens, because if $g(a_9) = 0$, then since $g(a_8) = 0$ we must have $g(a_7) = 1$. Hence, $g(a_1) = g(a_2) = g(a_3) = g(a_4) = 0$, so that $g(a_5) = g(a_6) = 1$, a contradiction.

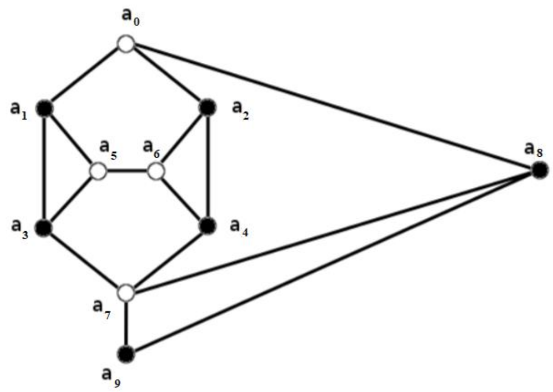


Fig. 2.3.4 A G_1 coloring that shows the contradiction

This means that if the instance of point a_0 of a copy of G_1 is "colored" with 1, then the instance of point a_9 of the same copy, also takes the value of 1. This observation, constitutes the backbone of proving Kochen and Specker theorem, because since the instance of a_9 of a copy is identified with the instance of a_0 in the neighboring copy, is implied that if one of these instances of point a_0 take the value of 1, then all the other instances of point a_0 must take the same value as well.

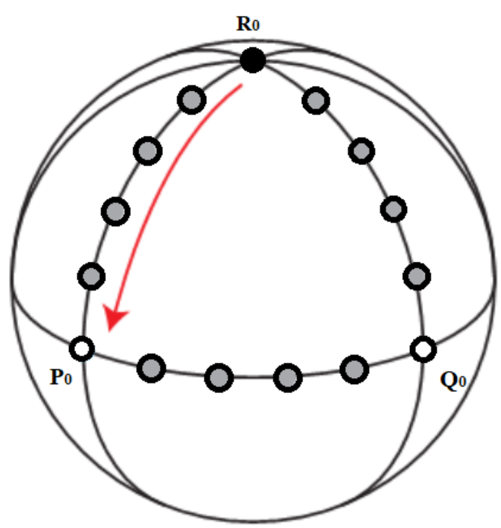


Fig. 2.3.5 Showing that each copy of a_0 should take the same color as the a_0 of the neighboring copy.

Now, since p_0, q_0, and r_0 lie in a triangle in G_2, exactly one of these points is mapped by g onto 1, say $g(r_0) = 1$. Hence, by the above argument we find $g(r_0) = g(r_1) = g(r_2) = g(r_3) = g(r_4) = g(p_0) = 1$. But $g(p_0) = 1$ contradicts the condition that $g(r_0) = 1$, and that proves the theorem.

□

This theorem implies that there is no map of the unit sphere S onto $\{0,1\}$ satisfying the condition (2.3.17), and hence no homomorphism from $\mathbb{B}(E^3)$ onto $\mathbb{Z}_2$. This result, can be obtained more simply either by a direct topological argument or by applying the Gleason's theorem [Gleason, 1957].

A system to apply the K-S theorem

Having proved that there is no embedding from the set of quantum propositions onto a Boolean algebra, we need to provide an example of a quantum system in which we can apply the K-S theorem. Let consider a qutrit, i.e. a system with a three dimensional associated Hilbert space, and more specifically a spin-1 system. In this case the "spin" can be described by the vector of the spin projection operators $\mathbb{S} = (S_x, S_y, S_z)$, where the directions of x, y and z be the direction of the usual three mutual orthogonal rays. In the usual representation, we have:

$$S_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad S_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

We can define the spin projector operator of the system, on the direction of the unit vector $\vec{v} \equiv (a, b, c)$, as $S_{\vec{v}} = \mathbb{S} \cdot \vec{v} = aS_x + bS_y + cS_z$, where of course $|a|^2 + |b|^2 + |c|^2 = 1$. One can easily show that the squares of the spin projector operators S_x, S_y, S_z are commuting:

$$[S_x^2, S_y^2] = [S_y^2, S_z^2] = [S_z^2, S_x^2] = 0 \tag{2.3.18}$$

And thus S_x^2, S_y^2, S_z^2 form a set of compatible observables.

Now, we will show that there is an embedding φ of the partial Boolean algebra $\mathbb{B}(E^3)$ into the partial Boolean algebra $\mathfrak{B}$ of quantum mechanical proposition. Let P be a projection operator belonging to a 3-dimensional eigenspace. For every 1-dimensional linear subspace v of E^3 there corresponds a spin projector operator S_v. We will define the φ as following: Let $\varphi(E^3) = P$ and $\varphi(0) = 0$. Now, let $\varphi(v) = PS_v^2$, for every 1-dimensional subspace v, and $\varphi(w) = P(\mathbb{1} - S_{w^\perp}^2)$, for every 2-dimensional subspace w, where the $w^\perp$ denotes the orthogonal complement of w. To show that φ is an embedding it clearly suffices to prove that if a and b are orthogonal 1-dimensional subspaces of E^3, then $[PS_a^2, PS_b^2] = 0$. But this is already true since

$$[PS_a^2, PS_b^2] = PS_a^2 PS_b^2 - PS_b^2 PS_a^2 = P(S_a^2 S_b^2 - S_b^2 S_a^2) = P[S_a^2, S_b^2] = P0 = 0$$

Note that the projection operator PS_a^2 is an element of $\mathfrak{B}$ and corresponds to the proposition P_a: "For every spin-1 system, the total angular momentum in the direction of a is not 0".

This concludes the proof of Kochen and Specker theorem.

2.4 KCBS inequality

As we have seen, the existence of an inequality which indicates contextual effects when violated, is extremely useful. The CHSH inequality for a system of two qubits, is such an example. The violation of CHSH indicates the existence of non-local correlations, which is a special case of contextual correlations on a paired system. Having the results of the K-S theorem in mind, we are going to present another inequality, that its violation indicates contextual correlations of the measurements on a single qutrit system, known as KCBS inequality (Klyachko et al 2008).

Let us consider a spin-1 system

Let consider a cyclic quintuplet of unit vectors $\{\ell_i\}_{i\in\mathbb{Z}_5}$ with $\ell_i \perp \ell_{i+1}$, $\forall\, i \in \mathbb{Z}_5$. We will call it a pentagram.

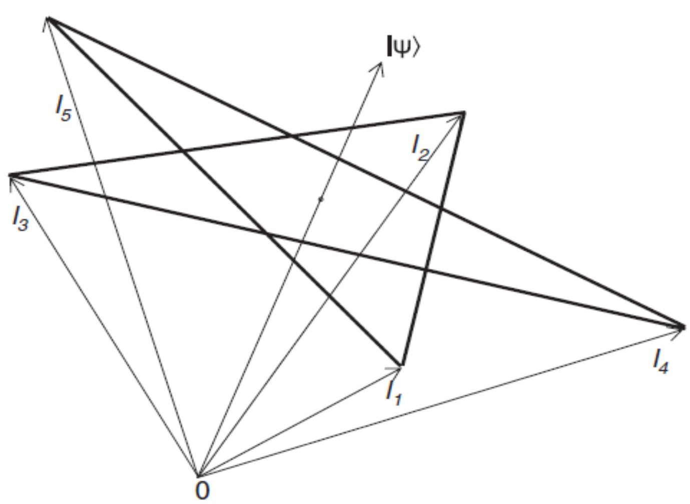
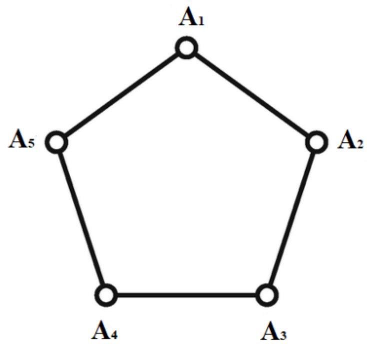


Fig. 2.4.1 Five cyclically orthogonal vectors in E^3

Also, consider the spin-1 vector $\mathbb{S} = (S_x, S_y, S_z)$ with

$$S_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and the spin projection operator $S_{\ell_i} = \mathbb{S} \cdot \ell_i$ onto the direction of ℓ_i. The orthogonality between the ℓ_i with successive indices, implies that the respective squares of S_{ℓ_i} commute:

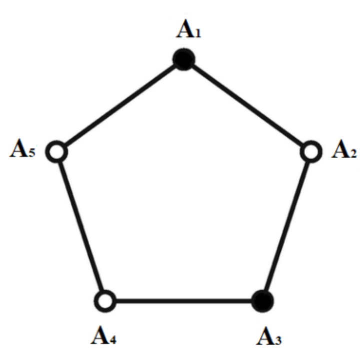


$[S_{\ell_i}^2, S_{\ell_{i+1}}^2] = 0\,,\ \forall\, i \in \mathbb{Z}_5$. Now, consider the observables $A_i = 2S_{\ell_i}^2 - \mathbb{1}$, since it is more convenient to deal with them due to the fact that each of them take values $a_i = \pm 1$. The relation of these observables can be represented by an exclusivity graph, where the vertices represent the observables and the edges represent the exclusivity relation between two compatible observables.

That means, after a measurement, these observables will give a positive value of +1 if the state of the system lies in their corresponding subspace, or -1 if it does not. However, due to the orthogonality relations, there cannot be two connected vertices that both take the value of +1 simultaneously. Knowing all that, we can construct the following polynomial:

$$a_1a_2 + a_2a_3 + a_3a_4 + a_4a_5 + a_5a_1 \qquad (2.4.1)$$

where the a_i denote the outcome of measuring observable A_i, and it is either +1 or -1. It is easy to show that the minimum value the polynomial (2.4.1) can take, satisfying the rule



of exclusivity above, is -3. Ideally, we would like all the monomials $a_i a_{i+1}$ to take the minimum value, that is -1, but something like that is impossible since at least two neighboring vertices have to take the value of -1 simultaneously, otherwise we would end up with two +1 neighboring vertices.

So, we have that:

$$a_1 a_2 + a_2 a_3 + a_3 a_4 + a_4 a_5 + a_5 a_1 \geq -3 \quad (2.4.2)$$

Assuming now the existence of a hidden variable joint distribution that would let our observables to take the a_i values simultaneously, we can take the respective expectation value of the relation (2.4.2). Thus we arrive at the inequality:

$$\text{(KCBS)} \quad \langle A_1 A_2 \rangle + \langle A_2 A_3 \rangle + \langle A_3 A_4 \rangle + \langle A_4 A_5 \rangle + \langle A_5 A_1 \rangle \geq -3 \quad (2.4.3)$$

We will call this inequality, KCBS or pentagram inequality, and its violation will indicate the absence of a hidden observable joint distribution, and the existence of contextual relations.

Now, we are going to give a set of observables that follows the above scenario, and thereafter we will find a vector state $|\psi\rangle$ that violates the KCBS inequality. Consider the following family of vectors:

$$|v_k\rangle = \cos\left(\frac{4k\pi}{5}\right)|0\rangle + \sin\left(\frac{4k\pi}{5}\right)|1\rangle + \sqrt{\cos\left(\frac{\pi}{5}\right)}\,|2\rangle \quad (2.4.4)$$

All these vectors are cyclically orthogonal similar to (Fig.2.4.1). Now, consider the following observables

$$A_i = 2\frac{|v_i\rangle\langle v_i|}{\langle v_i|v_i\rangle} - \mathbb{1} \quad (2.4.5)$$

The KCBS operator is:

$$KCBS = A_1 A_2 + A_2 A_3 + A_3 A_4 + A_4 A_5 + A_5 A_1 \quad (2.4.6)$$

If we take $|\psi\rangle = |2\rangle$ then the $\langle KCBS\rangle_2 = \langle 2|KCBS|2\rangle \cong -3.94427 < -3$

2.5 No Disturbance Principle

As we have mentioned in the Bell's inequality section, the Bell's factorizability condition is derived from a more fundamental principle called Principle of local causality.

Local causality states that any cause and effect between spatially separated systems is restricted by the velocity of light. However, multipartite quantum systems do not obey the principle of local causality, as the related experiments have shown. However there is a principle, similar to local causality, which poses less restrictions and the quantum theory indeed satisfies. This principle is called the No-Signaling (NS) principle and expresses the impossibility of sending information faster than a specific finite speed, and more specifically the speed of light. This principle is deeply rooted in our existing understanding of the physical world, and sets a more general framework in which we consider our current physical theories, and also restrict the structure of the possible future ones. This principle implies that the correlations between distant partners cannot be used to send information, as is the case for quantum correlations. Mathematically a correlation is expressed through a joint probability distribution $P(a,b|x,y)$, where a and b are outcomes of two separated parties, given that x and y are their free choices of measurement settings respectively. Therefore the non-signaling condition implies that the marginal probabilities are independent of the partner's choice: $P(a|x,y) = \sum_b P(a,b|x,y) = P(a|x)$. [Pawlowski 2009]

$$\text{(NS)} \qquad P(a|x,y) = \sum_b P(a,b|x,y) = P(a|x) \qquad (2.5.1)$$

However, there is an even more fundamental principle than NS, which any physical theory should satisfy: The No Disturbance Principle (ND)[Ramanathan et al 2012] is a generalization of the no-signaling principle that refers to compatible observables instead of space-like separated observables. To formulate the ND principle mathematically, let us consider a physical system on which one can perform several different measurements $A, B, C, \ldots$ etc. Let us assume that observables A and B are compatible, and also that A and C are compatible. That means that measurements on the observable pair A and B and on pair A and C can be jointly performed. This implies the existence of the joint probabilities $p(A=a, B=b)$ and $p(A=a, C=c)$, where a, b and c denote the outcomes of the corresponding measurements. The ND principle is the condition that the marginal probability $p(A=a)$ calculated from the joint distribution $p(A=a, B=b)$ is the same as that calculated from the $p(A=a, C=c)$. More specifically, the relation that holds is:

$$\text{(ND)} \qquad \sum_b p(A=a, B=b) = \sum_c p(A=a, C=c) = p(A=a) \qquad (2.5.2)$$

The ND principle is related to the fact that in any measurement experimental scenario, one may assign a probability value to each event independently of the context of measurement. Since this property is satisfied by any known physical theory, Quantum mechanics is not an exception. This principle initially formulated by Gleason [Gleason 1957], and thus we may also refer to it as Gleason's property.

3 Graph-theoretical approach to Contextuality.

3.1 Useful Graph-theoretical notions and theorems

As we saw on the Kochen – Specker proof, graph theory provides us with a suitable framework for describing any measuring scenario, and at the same time, equips us with a very useful theoretical "toolkit" for the study of non-local and contextual correlations. In the next sections we will provide graph theoretical description for many different experimental scenarios, while to approaching the notion of contextuality from a graph-theoretical point of view. However in order to do that we need to clarify some notions, provide definitions, and mention some important theorems we will use.

A graph is a structure amounting to a set of objects in which some pairs of the objects are in some sense "related". A simple undirected graph is a pair $G = \big(V(G), E(G)\big)$, where $V(G)$ is a set whose elements are called vertices, and $E(G)$ is a set of two-sets of vertices, i.e. $E(G) = \big\{\{x, y\}: x, y \in V(G)\big\}$, whose elements are called edges. From now on we will refer to simple undirected graphs simply as graphs. Now let give some useful definitions:

3.1.1 Definition

An induced subgraph of a graph G is another graph, formed from a subset of the vertices of G and all of those edges connecting pairs of vertices in that subset.

3.1.2 Definition

The complement of a graph G, is the graph $\bar{G}$ with the same vertex set but whose edge set consists of the edges not present in G.

3.1.3 Definition

Clique of a graph G is any complete subgraph of G.

3.1.4 Definition

We will call circuit graph, a graph that its edge set forms a path such that the first node of the path corresponds to the last.

3.1.5 Definition

We will call chordless cycle, or simply cycle, a circuit graph whose circular paths are all of the same length.

3.1.6 Definition

A maximal clique of a graph G, is a clique that cannot be extended by including one more adjacent vertex, meaning it is not a subset of a larger clique.

3.1.7 Definition

The clique number $\omega(G)$ of a graph G is the size of a maximum clique of G, i.e. the number of vertices in the largest maximal clique of G.

3.1.8 Definition

The chromatic number $\chi(G)$ of a graph G, is the smallest number of different colors needed to color the vertices of G so that two adjacent vertices never share the same color.

3.1.9 Definition

The vertex clique covering number $\theta(G)$ of a graph G is the minimum number of cliques in G needed to cover the vertex set of G.

3.1.10 Definition

Perfect graph is called a graph in which the chromatic number of every induced subgraph equals the size of the largest clique in that subgraph. Equivalently we can say that a graph G is perfect if and only if we have that $\chi(G[S]) = \omega(G[S])$, $\forall\, S \subseteq V(G)$, where $G[S]$ denotes induced subgraph of G with a vertex set S.

3.1.11 Weak Perfect graph theorem (Lovász 1972)

In graph theory, the perfect graph theorem states that an undirected graph G is perfect if and only if its complement graph $\bar{G}$ is also perfect.

3.1.12 Strong Perfect graph theorem (Chudnovsky et al. 2006)

The strong perfect graph theorem states that G is a perfect graph if and only if neither of G or $\bar{G}$ contains an induced cycle of odd length greater or equal to 5.

3.1.13 Lovász Sandwich Theorem (Lovász 1986)

The Lovász "sandwich theorem" states that the Lovász number of a graph always lies between the graph's clique number and the graph's chromatic number. More precisely:

$$\omega(G) \leq \vartheta(\bar{G}) \leq \chi(G) \tag{3.1.1}$$

3.1.14 Remark

Notice that in a graph G, a set of vertices is independent if and only if the corresponding vertices of the complement graph form a clique. That means that these two notions are complementary, and thus:

$$\alpha(G) = \omega(\bar{G}) \tag{3.1.2}$$

3.1.15 Theorem (Lovász 1979)

It is proved that the Lovász number $\vartheta(G)$ of a graph G provides an upper bound on the graph's Shannon capacity $\Theta(G)$, and therefore the following relation holds:

$$\alpha(G) \leq \Theta(G) \leq \vartheta(G) \tag{3.1.3}$$

3.1.16 Definition

The Shannon capacity $\Theta(G)$ of a graph G, is a graph invariant defined from the number of independent sets of strong graph products, namely:

$$\Theta(G) = \sup_{k} \sqrt[k]{\alpha(G^k)} = \lim_{k\to\infty} \sqrt[k]{\alpha(G^k)} \tag{3.1.4}$$

where G^k is the strong product of G with itself k times.

3.1.17 Remark

By coloring a graph G with $\chi(G)$ different colors, we basically perform a vertex decomposition into the fewer possible independent sets. Notice that these sets of vertices correspond to a clique decomposition with the fewer possible components of the graph complement $\bar{G}$. Hence, we conclude that the clique covering number of a graph is given by the chromatic number of its complement graph, and vice versa. Therefore:

$$\chi(G) = \theta(\bar{G}) \tag{3.1.5}$$

Now, we will proceed by formulating the basic framework for the study of the non-contextuality test inequalities.

3.2 Graphs for non-contextuality test inequalities

There are two types of graphs that can be associated to any measurement scenario and therefore to any given non-contextuality inequality [Cabello, 2010]. The first one consists of graphs that indicate the compatibility relations between a set of observables that we are interested in, and thus we call them compatibility graphs. The graph's vertices represent the observables that are measured in the experiment, while the edges denote the compatibility relation between the connected vertices, namely the ability to jointly measure the corresponding observables. Every possible subset of vertices that can be jointly measured, like a graph edge, is defining a measurement context or simply a context. The other type of graphs, called exclusivity graphs, are graphs that indicate the exclusivity relations between the outcome events regarding a measurement. Here the vertices represent events that may occur upon a measurement of a context, while the edges denote the mutual exclusivity relation between the event-vertices they connect. The events which are represented by vertices, usually take the form $\{A_{i_1} = a_{i_1}, \dots, A_{i_k} = a_{i_k}\}$ or $\{a_{i_1}, \dots, a_{i_k} | A_{i_1}, \dots, A_{i_k}\}$, meaning that for a context defined by $(A_{i_1}, \dots, A_{i_k})$, which is a set of pairwise compatible observables we measure simultaneously, the outcome of measurement for the observable A_{i_j} is a_{i_j} for every $j = 1, \dots, k$. In many cases, an event occurring in a composite system may be expressed as $\{x_i, x_j, \dots | i, j, \dots\}$, where x_i is referring to the outcome of measuring the i-th observable of the first subsystem, x_j is referring to the outcome of measuring the j-th observable of the second subsystem and so on. For example, in a Bell-type scenario, with $P(a, b|i, j)$ we denote the probability of the event "the result a has been obtained when measuring A_i, and the result b has been obtained when measuring B_j", while with $P(A_i = a)$ we denote the probability of the event "the result obtained for measuring A_i was a". For a given experimental scenario, we can use either the exclusivity graph of all possible events or any of the induced subgraphs of this graph in order to derive a noncontextual inequality. From now on we will be referring to the exclusivity graph of all possible events as global exclusivity graph of the scenario, while any of the induced subgraphs will be simply labeled as exclusivity graph. When we construct noncontextual inequalities we usually use dichotomic observables, namely observables that take two distinct values, which in quantum mechanics represent the binary answer to the question "if the post measuring state of the system lies in a specific linear subspace of the system's associated Hilbert space". From now on, we will mainly consider as possible outcomes for measuring an observable either the values $\{0,1\}$, or $\{-1,1\}$, depending on our objective. Now let see some useful examples about compatibility and exclusivity graphs.

CHSH scenario's graphs

One of the most well-known quantum-theoretical set-ups is the Bell scenario, where measurements performed in a pair of two entangled qubits. In this scenario we have two measurement settings for each qubit subsystem; let say A_0, A_1 for the first qubit and B_0, B_1 for the second. The observables take the values $\{-1,1\}$ upon measurement and every observable of the first system is compatible with every observable on the second one, while none of the observables on the same system are compatible with each other. This set-up can be described by the following two graphs:

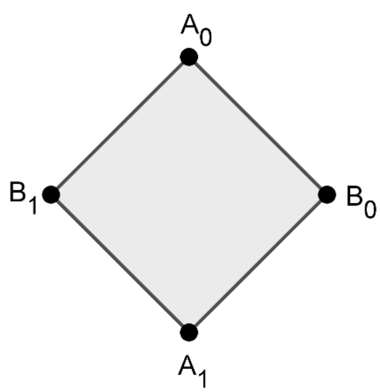


Fig.3.2.1 Compatibility graph of the CHSH scenario

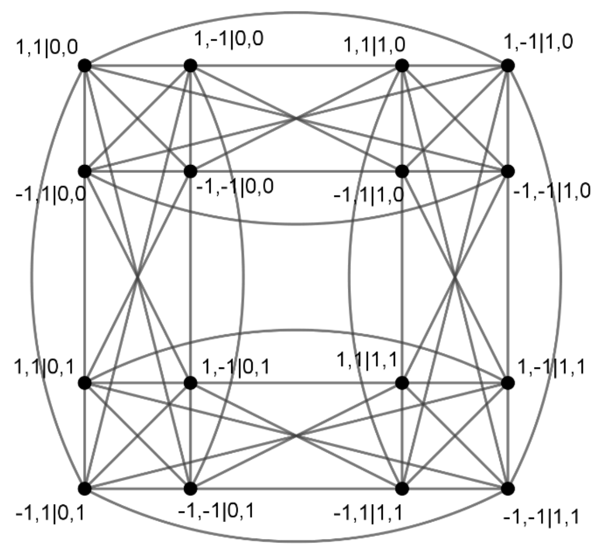


Fig.3.2.2 Global Exclusivity graph of the CHSH scenario

The exclusivity relations of the exclusivity graph arise from the acceptance that the no-signaling principle holds, which is a special case of a more general principle that governs Quantum theory, the No-Disturbance (ND) principle. In other words, if we measure a context that corresponds to A_i and then a different context that also corresponds to A_i we must find the same outcome a_i in both cases. That means that the events $\{1, a|i, j\}$ and $\{-1, b|i, k\}$ are disjoint. However, for constructing the corresponding inequality, we make use of an induced subgraph of the global exclusivity graph like the following [Cabello et al, 2014]:

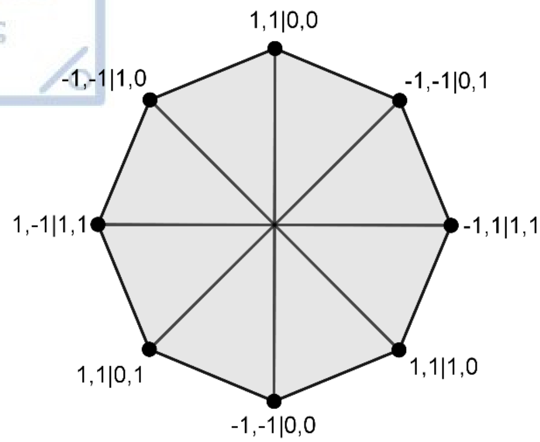


Fig.3.2.3 CHSH exclusivity graph used for the derivation of the inequality.

KCBS scenario's graphs

Another important quantum-theoretical set-up is the KCBS scenario, which is related to the fact that a quantum system with an associated Hilbert space of dimension three or higher displays contextual "behavior". The default KCBS inequality refers to a qutrit system, and is formulated by making use of five cyclic compatible dichotomic observables which take the values $\{0,1\}$ (or $\{-1,1\}$, it depends from our objective) upon measurement. The compatibility relations between the observables can be seen in the graph below.

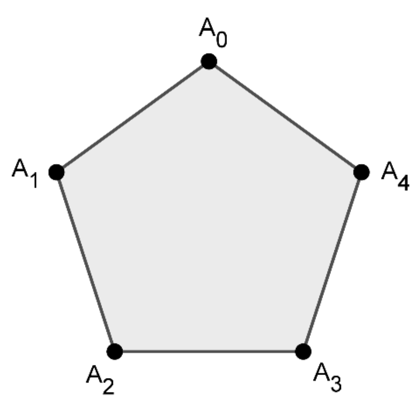


Fig.3.2.4 KCBS scenario's Compatibility graph

As we have seen, the observables in a KCBS scenario represent 1-dimensional subspaces of the system's associated Hilbert space that are successively orthogonal. Therefore, two orthogonal subspaces not only correspond to compatible observables but they also correspond to mutual exclusive events. That means that two consecutive observables A_i and A_{i+1}, with respect to modulo 5 addition, can never take the value 1 at the same time. Therefore, we can construct the following two exclusivity graphs depending on the observables we jointly measure.

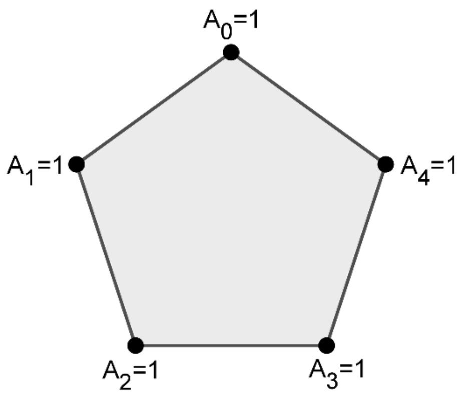


Fig.3.2.5 KCBS exclusivity graph for the measurement of Ai

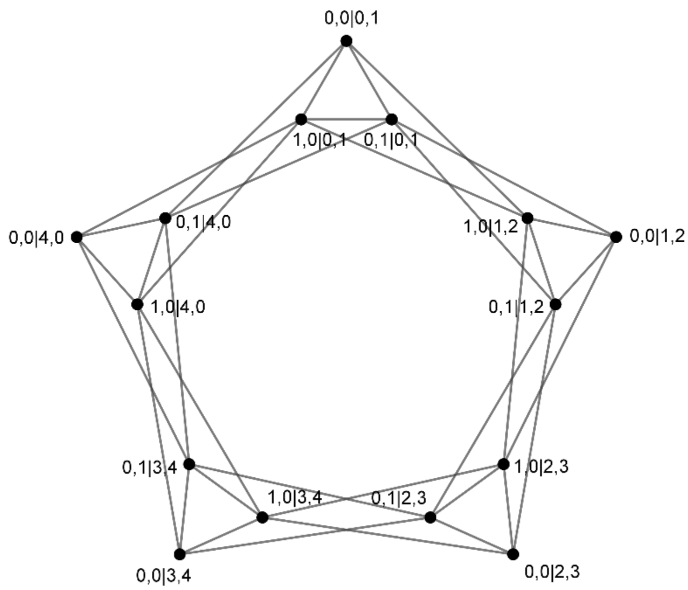


Fig.3.2.6 KCBS exclusivity graph for the joint measurement (Ai,Ai+1)

However, for the formulation of the corresponding inequalities, we use either the graph with the measurements of $\{A_i\}$, or the following induced subgraph of the case we jointly measure on a context defined by $\{A_i, A_{i+1}\}$:

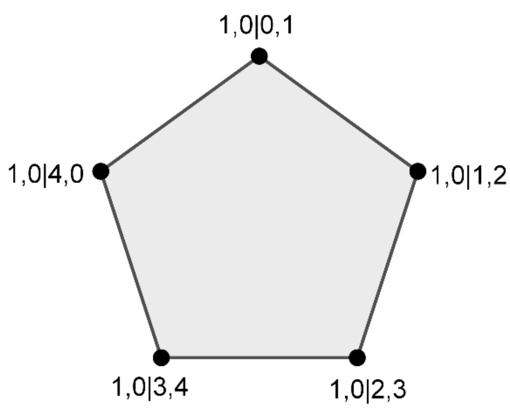


Fig.3.2.7 Exclusivity graph of the KCBS inequality. It is an induced subgraph of the graph in Fig.#

Note, that because of the mutual exclusiveness of the compatibility relations, the exclusivity graphs of (Fig.3.2.5) and (Fig.3.2.7) end up the same with the compatibility graph. For this reason, one may find cases in literature, where the non-contextual bound of a KCBS type inequality is derived directly from the compatibility graph.

3.3 Deriving the non-contextual bounds and constructing the inequalities

In order to derive a non-contextuality test inequality, we need to determine an upper or a lower bound of a specific expression, beyond which, the existence of noncontextual correlations is impossible. As we have said before, a non-contextual model would require the existence of a joint probability distribution over all the observables we measure. This means, that the occurrence of any event appearing in the expression's exclusivity graph, would prevent the occurrence of all the events which are disjoint with it, namely all the events that are connected to it via an edge that indicates exclusivity. Therefore the maximum number of events that can occur in a noncontextual model are given by the maximum number of pairwise nonadjacent vertices in the scenario's exclusivity graph, i.e. the graph's independence number [Cabello et all 2014]. By applying the mutual exclusivity principle on the scenario's events, we further get that the total sum of the probabilities corresponding to these events must be at most equal to the graphs independence number.

For instance, if G_{CHSH} and G_{KCBS} are the exclusivity graphs of the CHSH and KCBS scenarios, illustrated in figures (3.2.3) and (3.2.5), the non-contextual bounds for the corresponding inequalities are $\alpha(G_{CHSH}) = 3$ and $\alpha(G_{KCBS}) = 2$ respectively. That makes the noncontextual inequalities to take the following form:

(CHSH) $$P(1,1|0,0) + P(-1,-1|0,0) + P(1,1|0,1) + P(-1,-1|0,1) + P(1,1|1,0) + P(-1,-1|1,0) + P(1,-1|1,1) + P(-1,1|1,1) \underset{NCHV}{\leq} 3 \quad (3.3.1)$$

(KCBS) $$\sum_{i=1}^{5} P(A_i = 1) \underset{NCHV}{\leq} 2 \quad (3.3.2)$$

These expressions can easily be restated into the more familiar forms of:

(CHSH) $$\langle A_0B_0\rangle + \langle A_0B_1\rangle + \langle A_1B_0\rangle - \langle A_1B_1\rangle \underset{NCHV}{\leq} 2 \quad (3.3.3a)$$

or equivalently

(CHSH) $$\langle A_0B_0\rangle + \langle A_0B_1\rangle + \langle A_1B_0\rangle - \langle A_1B_1\rangle \underset{NCHV}{\geq} -2 \quad (3.3.3b)$$

for the CHSH inequality; and into the form

(KCBS) $$\langle A_1A_2\rangle + \langle A_2A_3\rangle + \langle A_3A_4\rangle + \langle A_4A_5\rangle + \langle A_5A_1\rangle \underset{NCHV}{\geq} -3 \qquad (3.3.4)$$

For the KCBS inequality, by using the probabilities appearing on the expressions (3.3.1) and (3.3.2) in order to derive the corresponding expected values.

For instance, for the CHSH scenario, by taking into account that

$$\langle A_iB_j\rangle = P(1,1|i,j) + P(-1,-1|i,j) - P(-1,1|i,j) - P(1,-1|i,j) \qquad (3.3.5)$$

And also that

$$P(1,1|i,j) + P(-1,-1|i,j) + P(-1,1|i,j) + P(1,-1|i,j) = 1 \qquad (3.3.6)$$

one may write the expected value $\langle A_iB_j\rangle$ as following:

$$\pm\langle A_iB_j\rangle = 2[P(1,\pm1|i,j) + P(-1,\mp1|i,j)] - 1 \qquad (3.3.7)$$

From this, we can easily rewrite the relation (3.3.1) in the form (3.3.3a). The expression (3.3.3b) can be derived in a similar manner with the above, if we consider a different induced subgraph of the original exclusivity graph that contains all possible events. For instance if we choose to derive our inequality from the following exclusivity graph:

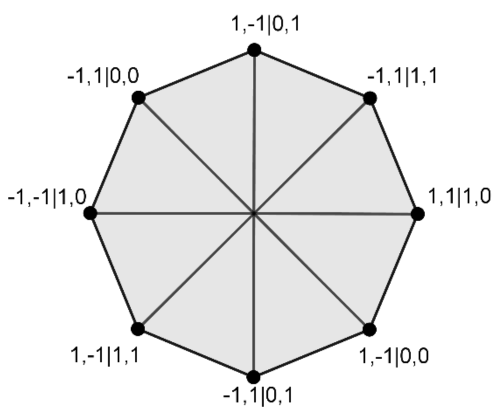


Fig. 3.3.1 A CHSH exclusivity graph of (3.3.3b) type

which is also an induced subgraph of the global exclusivity graph, we would end up with the following probability inequality:

(CHSH) $$\begin{aligned} &P(1,-1|0,1) + P(-1,1|1,1) + P(1,1|1,0) + P(1,-1|0,0) + P(-1,1|0,1) \\ &+ P(1,-1|1,1) + P(-1,-1|1,0) + P(-1,1|0,0) \underset{NCHV}{\leq} 3 \end{aligned} \qquad (3.3.8)$$

And thus with the relation (3.3.3b).

On the other hand, for the KCBS scenario, we need to consider the case where we are using $\{-1,1\}$ as the possible outcomes of the dichotomic observables. We may also use the following expression instead of the expression (3.3.2):

$$\text{(KCBS)} \qquad \sum_{i=1}^{5} P(1,-1|i,i+1) \underset{NCHV}{\leq} 2 \qquad (3.3.9)$$

These two relations are equivalent, since from the ND principle and the mutual exclusiveness indicating by the compatibility graph, is implied that $P(A_i = 1) = P(1,-1|i,i+1)$. Now, one may write the expected value $\langle A_i A_{i+1}\rangle$ as:

$$\langle A_i A_{i+1}\rangle = P(-1,-1|i,i+1) - P(1,-1|i,i+1) - P(-1,1|i,i+1) \qquad (3.3.10)$$

Also notice that upon a joint measurement $\{A_i, A_{i+1}\}$, the relation

$$(-1,-1|i,i+1) + P(1,-1|i,i+1) + P(-1,1|i,i+1) = 1 \qquad (3.3.11)$$

holds, since $\{A_i = 1, A_{i+1} = -1\}$, $\{A_i = -1, A_{i+1} = -1\}$ and $\{A_i = -1, A_{i+1} = 1\}$ are all the possible disjoint events that may occur. Considering that, we can write

$$\langle A_i A_{i+1}\rangle = 1 - 2[P(1,-1|i,i+1) + P(-1,1|i,i+1)] \qquad (3.3.12)$$

By summing up the expectation values of all five 2-sets of successively compatible observables, we obtain

$$\sum_{i=1}^{5}\langle A_i A_{i+1}\rangle = 5 - 4\sum_{i=1}^{5} P(1,-1|i,i+1) \qquad (3.3.13)$$

And from here, one can easily conclude that

$$\text{(KCBS)} \qquad \sum_{i=1}^{5}\langle A_i A_{i+1}\rangle \underset{NCHV}{\geq} -3 \qquad (3.3.14)$$

Which is exactly the relation (3.3.4).

3.4 Probability assignment and inequality's maximum violation

Consider a scenario described by a compatibility graph G. If $C \subseteq V(G)$ is a vertex set that corresponds to a measurement context of G, we can assign a joint probability distribution on C and therefore we can assign a probability p_i to each vertex $v_i \in C$ given that we are measuring the context C. However, if our theory satisfies the ND principle, we can assume that the marginal probability p_i of the vertex v_i should be the same independently of the context it came from. Therefore, we can assign a probability p_i, independently of context, on every vertex v_i of the graph G. Notice that upon a context's C measurement, the events these probabilities are representing are pairwise disjoint, since at most one outcome $i \in C$ can occur. Thus the following condition must be satisfied:

$$\sum_{i \in C} p_i = 1 \tag{3.4.1}$$

Also notice that this probability assignment is not necessary unique, and there can be many possible assignments that satisfy the above conditions. From now on, we will refer to such a probability assignment as a probabilistic model of the scenario with compatibility graph G.

***3.4.1 Definition** (Acín et al, 2015)*

Let G be compatibility graph of a contextuality scenario. A probabilistic model on G is an assignment $p : V(G) \to [0,1]$ of a probability $p(v)$ to each vertex $v \in V(G)$ such that

$$\sum_{v \in C} p(v) = 1 \quad \forall\, C \tag{3.4.2}$$

where C is a measuring context of G.

Notice, that for any subset of the set of vertices that corresponds to a context, such as an edge of the compatibility graph, the following is true:

$$\sum_{v \in e} p(v) = 1 \quad \forall\, e \in E(G) \tag{3.4.3}$$

All the possible probabilistic models of a scenario G, can be represented as a convex polytope in the n-dimension Euclidean space, defined by the aforementioned inequalities.

In the case of Quantum mechanics, this probability assignment is achieved through a set of rank-1 projection operators P_i which correspond to the event that "the post measuring state lies on the Hilbert ray represented by vertex v_i". The eigenvalues of these projectors are either 0 or 1, and thus they can be considered as binary propositions [Cabello et al, 2010].

Consider for example a contextual testing scenario, and its corresponding exclusivity graph G. Each one of the events $\mathcal{E}_i$ which is presented in this scenario, is associated with a projection operator P_i which indicates whether or not the event $\mathcal{E}_i$ occurs by giving the truth values 0,1 upon measurement. For a given state $|\psi\rangle$, the expectation value $\langle P_i\rangle_\psi = \langle\psi|P_i|\psi\rangle$ provide us with the probability of the event $\mathcal{E}_i$ to occur. This assignment of $\langle P_i\rangle_\psi$ to every vertex is a probabilistic model of G that depends on the initial state $|\psi\rangle$. Notice that this assignment of probabilities is independent of the context. This condition, is the one that underlies Gleason's theorem [Gleason, 1957], and thus we call it Gleason property. Since this assignment is a probabilistic model, from (3.4.3) is implied that for every edge $\{i,j\}$ of the exclusivity graph G the following must be true:

$$\langle P_i\rangle_\psi + \langle P_j\rangle_\psi \leq 1\,, \forall(i,j) \in E(G), \forall|\psi\rangle \in \mathcal{H}^* \implies P_i + P_j \leq \mathbb{1} \qquad (3.4.4)$$

Therefore, the condition that underlies a quantum probabilistic model is: $P_i + P_j \leq \mathbb{1}$.

By summing up all the expectation values $\langle P_i\rangle$, we get:

$$\beta_\psi = \sum_{i\in V(G)} \langle P_i\rangle_\psi \qquad (3.4.5)$$

Note that this expression is basically our non-contextuality test operator. Since all the possible probabilistic models lie in a convex polytope on an n-Euclidean space, it is easy to conclude that the expression (3.4.5) takes its maximum value on an extremal point of the polytope.

As we have seen, each exclusivity graph G gives rise to a non-contextual inequality with a non-contextual bound equal to the graphs independence number $\alpha(G)$. The violation of that inequality implies a non-contextual correlation, as well as the inability to construct a joint distribution over all our variables. However, a reasonable question that may arise, is which the maximum possible violation for such an inequality is. The answer is that the maximum possible violation is given by the exclusivity graph's G Lovász number $\vartheta(G)$ (Cabello 2010). First, let us define the Lovász number $\vartheta(G)$ of a graph G:

3.4.2 Definition (Cabello 2010)

An orthogonal representation (OR) of a graph G, is a set of unit vectors associated to the vertices such that two vectors are orthogonal iff the corresponding vertices are adjacent.

3.4.3 Definition (Cabello 2010)

The Lovász number $\vartheta(G)$ of graph G is defined as the following maximum value:

$$\vartheta(G) = \max_{|\psi\rangle, V} \sum_{i=1}^{n} |\langle\psi|v_i\rangle|^2 \qquad (3.4.6)$$

where the maximum is taken over all unit vectors $|\psi\rangle$ in the n-dimensional Euclidean space $\mathbb{E}^n$ and over all possible ORs $V = \{|v_i\rangle : i \in \{1, .. n\}\}$ of G. Without loss of generality it suffices to consider the dimension n of the $\mathbb{E}^n$ to be equal to the number of graph's vertices.

To prove that the Lovász number determines the maximum possible value that a test operator can take, we need to make a few notices. First, notice that for a given probabilistic model, the expectation value is always maximized on an extremal point of the associated polytope i.e. on a pure state. Let the maximizing state be $|\psi\rangle$. Then, notice that for each projector operator P_i that assigns the probability $\langle P_i\rangle_\psi = \langle\psi|P_i|\psi\rangle$ to the vertex i, we can choose a suitable unit vector $|v_i\rangle$, given by $|v_i\rangle := \frac{P_i|\psi\rangle}{\sqrt{\langle\psi|P_i|\psi\rangle}}$, such that the expectation value $\langle P_i\rangle_\psi$ can be written as $\langle P_i\rangle_\psi = |\langle\psi|v_i\rangle|^2$. Actually that makes the operators P_i to be the projectors $|v_i\rangle\langle v_i|$. This collection of $|v_i\rangle$, is in fact an orthogonal representation of G, and the maximum value of β_ψ is given by the previous definition of the Lovász number.

3.5 Some observations about the quantum contextuality graphs

As we have seen until now, we can associate any experimental scenario of quantum theory to an exclusivity graph G, where the non-contextual bound is provided by the graph's independence number $\alpha(G)$, while the maximum contextual violation, or the ND-bound, is given by the graph's Lovász number $\vartheta(G)$. We can distinguish the exclusivity graphs into two classes, and thus the experimental scenarios into two categories. First, we have the graphs G for which $\alpha(G) < \vartheta(G)$. These graphs clearly allow a violation of the non-contextual bound and hereafter we will refer to them as contextual graphs (CG). The second class, constitutes of those graphs G for which $\alpha(G) = \vartheta(G)$. Since the upper bound of these graphs is the same as their non-contextual bound, they do not permit the appearance of contextual correlations, and therefore we will call them non-contextual graphs (NCG). From a probabilistic point of view, the NCGs permit the construction of a joint probability distribution for the observables' outcomes, while the CGs do not allow the existence of a model that can be explained through a joint probability distribution.

Having in mind the graph-theoretic notions and theorems we mentioned previously, we will proceed by proving a theorem and making some remarks about the contextuality graphs.

3.5.1 Theorem (Cabello et al 2012)

Let G be the exclusivity of a non-contextuality inequality. If G is a perfect graph, then G is a NCG and, as consequence, the inequality is never violated by Quantum Theory.

Proof

If G is perfect, then by definition $\omega(G) = \chi(G)$. On the other hand, according to Lovász sandwich theorem we know that $\omega(G) \leq \vartheta(\bar{G}) \leq \chi(G)$ for any graph G. Hence, G being perfect implies that $\omega(G) = \vartheta(\bar{G}) = \chi(G)$. Given that $\omega(G) = \alpha(\bar{G})$, we obtain that $\alpha(\bar{G}) = \vartheta(\bar{G})$, which means that if G is perfect, then $\bar{G}$ is NCG. From the weak perfect graph theorem, we obtain that since G is perfect, then $\bar{G}$ is perfect too. Therefore, by repeating the previous argument the other way around we conclude that G is a NCG as well. This finishes the proof.

□

3.5.2 Corollary 1 (Cabello et al 2012)

From the previous proof, we can also derive the more general conclusion: if G is a perfect graph, the $\alpha(G) = \vartheta(G)$.

3.5.3 Corollary 2 (Cabello et al 2012)

If G is the exclusivity graph of a non-contextual inequality that can be violated by Quantum theory, namely a CG, then G is not perfect. Consequently, by the strong perfect graph theorem, G must contain odd cycles and/or odd anti-cycles as induced subgraphs.

3.5.4 Remark 1 (Cabello et al 2012)

Notice that there could be a case in which a non-contextuality inequality is never violated by the Quantum theory, but at the same time it contains another non-contextuality inequality which can be violated by Quantum theory. This means that even if the exclusivity graph of the initial inequality is a NCG, there may be induced subgraphs of this graph that are CG.

3.5.5 Remark 2

No odd cycle or a complement of an odd cycle has another odd cycle or complement of an odd cycle as an induced subgraph. This suggests that odd cycles and their complements could be used as a basis for an exclusivity graph decomposition.

Now we can also prove another proposition about the perfect graphs, which is going to be useful later:

3.5.6 Proposition

If G is a perfect graph, then its independence number is equal to its vertex clique covering number , i.e. $\alpha(G) = \theta(G)$.

Proof

From the weak perfect graph theorem we have that, since $\bar{G}$ has to be perfect, since G is a perfect graph. Similarly to the proof of (3.5.1), we can show that $\bar{G}$ being perfect implies that $\omega(\bar{G}) = \vartheta(G) = \chi(\bar{G})$. However, we already know that $\chi(\bar{G}) = \theta(G)$, and thus $\vartheta(G) = \theta(G)$. Because G is perfect, from (3.5.2), we also know that $\alpha(G) = \vartheta(G)$. Hence, we obtain that $\alpha(G) = \theta(G)$ for every perfect graph G.

□

4 About Contextuality Monogamy

Inequalities like the KCBS are violated in any contextual theory such as Quantum Theory, where a joint probability distribution over all observables does not exist. The satisfaction of the KCBS inequality constitutes a necessary and sufficient condition for the existence of a non-contextual model that describes the scenario's set of five observables. Knowing that Quantum theory is a contextual theory that satisfies the No – Disturbance principle, a natural question arises: Is there a monogamy relation between two different non-contextuality test inequalities that correspond to the same, or to different interacting quantum systems? Seemingly, the answer is positive, therefore we will proceed by presenting a general way to derive a monogamy relations, and then we will provide an example of a KCBS inequality monogamy which is derived from the ND principle [Ramanathan et al, 2012], in a similar way in which Bell inequalities monogamy derived from the No – Signaling principle [Pawloski et al, 2009].

Before presenting the method of the contextual monogamy identification, we need to clarify what exactly we mean when we say: "monogamy relation between non-contextual inequalities".

Definition of Monogamous Contextuality (Ramanathan et al. 2012)

We will define as Contextual Monogamy the following: A set of measurements is said to have *monogamous contextuality* if it can be partitioned into disjoint subsets, each of which can by themselves reveal contextuality, but they cannot all simultaneously be contextual. In the case of locality and non-contextuality test inequalities, is implied that there are at least two disjoint sets of observables on the same system from which exactly one violates its corresponding test inequality.

4.1 A generalized method to derive monogamy relation for contextuality inequalities.

In order to acquire a better understanding about the mechanisms that govern the quantum contextuality, we are going to present a generalized method for deriving monogamy relations for contextual and non-local inequalities by using some graph-theoretic notions. This method was initially illustrated by Ramanathan et al. in their paper: "Generalized Monogamy of contextual inequalities from the no-disturbance principle".

First, we need to define some notions and prove some statements.

4.1.1 Definition

A graph G is called chordal if every cycle of length four or more in G has a chord in G. Equivalently, we can say that a chordal graph is a graph that does not contain an induced cycle of length greater than 3.

4.1.2 Remark

Chordal graphs is a specific case of perfect graphs.

4.1.3 Proposition

Every three connected vertices in a compatibility graph produce a joint probability distribution.

Proof:

First, notice that the set of events that correspond to an edge measurement, forms a clique on the scenario's exclusivity graph. By constructing the exclusivity graph that corresponds to the measurement of two neighboring edges of the compatibility graph, one can easily see that the largest hole or anti-hole that this graph contains is of length 4.

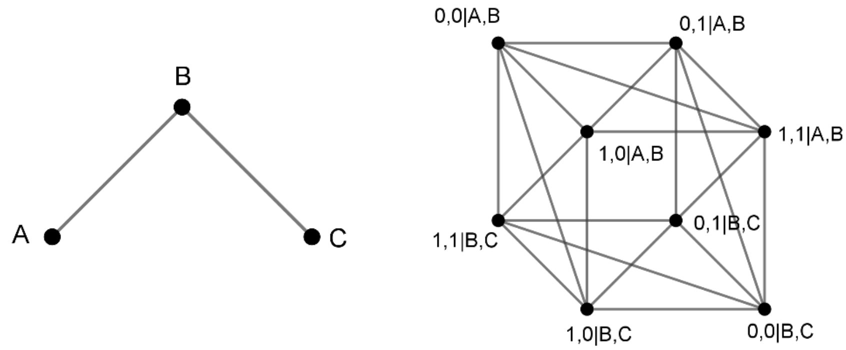


Fig. 1 The compatibility graph (left) and the corresponding exclusivity graph (right), for the case of three dichotomic observables.

That is also true for any compatibility's graph triangle, since any collection of events distributed in the different context cliques, would result in a 4-length hole or anti-hole at most.

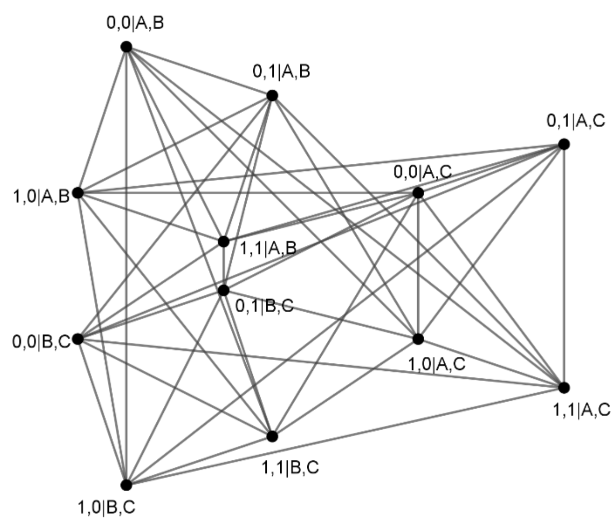


Fig. 2 The exclusivity graph of a compatibility triangle of three dichotomic observables. The largest induced cycle is of length 4.

According to (3.5.3), this implies that any three connected vertices in a compatibility graph can be measured in the same context and induces a joint probability distribution.

□

Any induced cycle of a chordal subgraph has a exactly length 3. That means that we are able to decompose every chordal graph into connected 3-cliques which induce a joint distribution, and that the corresponding exclusivity graph will have at most 4-legth holes and anti-holes. The probability distribution construction is explained with the following proposition.

4.1.4 Proposition (Ramanathan et al. 2012)

Any chordal compatibility graph G representing a set of n measurements, admits a joint probability distribution for these measurements.

Proof:

By assumption, we have that compatibility graph G does not contain any induced cycles of length greater than three. Let us denote the set of vertices of G by $V(G) = \{v_1, \dots, v_n\}$. Now let us define the following collections of subsets of $V(G)$: With K_3 we will denote the set of cycles of length 3 or more in G, i.e. $K_3 = \left\{K_3^{(i)}\right\}_{i \in I_3}$, where $K_3^{(i)} \in \bigcup_{k\geq 3}\big(V(G)\big)^k$, such that the vertices belonging to $K_3^{(i)}$ are defining a cycle. With K_2 we will denote the set of edges of G that are not subgraphs of any graph $K_3^{(i)}$, i.e. $K_2 = \left\{K_2^{(i)}\right\}_{i \in I_2}$, where $K_2^{(i)} \in E(G) = V^2(G) = V(G) \times V(G)$ and $\nexists j \in I_3 : \ K_2^{(i)} \subseteq K_3^{(j)}$. With K_1 we will denote the set of vertices of G that are not subgraphs of any graph $K_3^{(i)}$ or $K_2^{(j)}$, i.e. $K_1 = \left\{K_1^{(i)}\right\}_{i \in I_1}$, where $K_1^{(i)} \subseteq \big\{\{v\} : v \in V(G)\big\}$ and $\nexists (j,k) \in I_2 \times I_3 : \ K_1^{(i)} \subseteq K_2^{(j)} \ or \ K_1^{(i)} \subseteq K_3^{(k)}$. Notice that these three sets induce a partition of the set of edges of G, since each one of the edges of a chordal graph belongs to one and only one of the sets K_1, K_2, K_3. However, an edge may be appear multiple times within a set K_i as a subset of its elements, while the vertices of G may appear multiple times on different sets. Let $K = K_1 \cup K_2 \cup K_3$. We construct the joint probability distribution for the set of n measurements in G as following:

$$P(v_1, \dots, v_2) = \frac{\prod_{i=1}^{|K_3|} \prod_{j=1}^{|K_2|} \prod_{k=1}^{|K_1|} P\left(K_3^{(i)}\right) P\left(K_2^{(j)}\right) P\left(K_1^{(k)}\right)}{\prod_{i<j=1}^{|K|} P(K^{(i)} \cap K^{(j)})^{[\![K^{(i)} \cap K^{(j)} \neq \emptyset]\!]}} \tag{4.1.1}$$

Where $|A|$ denotes the cardinality of the set A and $P\big(K^{(i)} \cap K^{(j)}\big)^{[\![K^{(i)} \cap K^{(j)} \neq \emptyset]\!]}$ denotes the probability of the set of vertices that are at the intersection of the two elements $K^{(i)}$ and $K^{(j)}$ in the case where $K^{(i)} \cap K^{(j)} \neq \emptyset$. For any element $K^{(i)} \in K$ we can derive a marginal probability distribution $P\big(K^{(i)}\big)$ from the joint probability distribution by summing over all elements of K other than $K^{(i)}$. This summation over the elements $K^{(j)} \in K \setminus \left\{K^{(i)}\right\}$ is performed starting out starting with those elements $K^{(j)}$ which are disjoint with $K^{(i)}$, i.e. $K^{(i)} \cap K^{(j)} \neq \emptyset$. One can immediately see that in the resulting expression after that first summation all the terms in the denominator $\prod_{i<j=1}^{|K|} P\left(K^{(i)} \cap K^{(j)}\right)$ precisely cancel with all the terms in the numerator except for $P\left(K^{(i)}\right)$. That completes our constructive proof.

□

This proposition basically suggests that any measuring scenario that is described via a chordal compatibility graph forbids the construction of a contextual model that violates the non-contextual bounds. We are going to use this interesting fact in order to formulate a method for the derivation of monogamy relations between contextuality inequalities (Ramanathan et al 2012). Given a compatibility graph that represents a set of n noncontextual inequalities, where R is their non-contextual bound, we are going to look for a vertex decomposition into m chordal subgraphs, each of which admits a joint probability distribution, such that the sum of the corresponding NC-bounds of these subgraphs is equal to $n \cdot R$. If however the inequalities are not the same and have different bounds, let say n_1 of them have a non-contextual bound R_1, n_2 of them have a non-contextual bound R_2, … , and n_k of them have a non-contextual bound R_k, then we will try to choose the subgraphs such that the sum of their independence number is $\sum_k n_k R_k$. Note that each one of the vertices of the initial compatibility graph have to be included into a chordal subgraph of the decomposition, with no vertex appearing in more than one subgraph, while the edges between different subgraphs may be neglected. If we are able to carry out a vertex decomposition like this, we end up with a monogamy relation between the initial n noncontextual inequalities. That is, because only one of them may be violate its corresponding non-contextual bound while preserving the system's total restrictions imposed by the chordal subgraph decomposition. Note, that in the case where some vertices belong to multiple noncontextual inequality scenarios, we have to take account of the vertex multiplicity, i.e. we need to include this vertex as many times as the number of the inequalities it belongs, in order to perform the aforementioned decomposition.

Let be a little more enlightening about why is that true. As we have seen, the ND principle allows us to construct joint probability distributions and at the same time ensures us that the measuring probability of each observable is the same whether it is derived from a joint probability of a chordal subgraph component or from measuring the contexts given by the edges of the compatibility graph. We also know that there is a noncontextual relation between the observables of a chordal subgraph, since every such subgraph emits a joint probability distribution. That implies that the observables of a theory satisfying the ND principle would never violate the non-contextual bound of the chordal subgraph that they belong. For the case of an KCBS-type scenario this bound is the independence number of this particular subgraph. As an immediate corollary of that, we have that the total sum of the observable probability distributions must be bounded by the sum of all the non-contextual bounds of the n inequalities we have begun with. But since the graph vertices can also be decomposed into the corresponding subgraphs of the n inequalities, is implied that at most one contextual inequality can be violated and satisfy the previous restriction imposed by ND principle at the same time. Thus we have a monogamy relation between those non-contextuality test inequalities.

Note, that while many contextual inequalities involve rank-1 projectors and thus the edges of the corresponding compatibility graphs denote also a mutual exclusiveness relation, this assumption is not necessary for the derivation of monogamies. A representative example is the derivation of the Bell inequality monogamy (4.4).

4.1.5 Proposition (Ramanathan et al. 2012)

Consider a compatibility graph representing a set of n KCBS-type contextual inequalities each of which has non-contextual bound R. Then, this graph gives rise to a monogamy relation using the outlined method if and only if its vertex clique cover number is $n \cdot R$.

Proof:

Let G be a compatibility graph representing a system which contains n KCBS-type inequalities $K_j \leq R$, $j = 1,2,\dots,n$, with non-contextual bound R. The condition that the vertex clique covering number is $n \cdot R$ is clearly sufficient for the existence of monogamy, as each clique has independence number of 1, and cliques are the only graphs with independence number 1. Thus, a vertex decomposition of the compatibility graph into n cliques gives rise to the monogamy relation $\sum_{j=1}^{n} K_j \leq nR$.

Therefore there exists one decomposition into subgraphs that gives rise to a monogamous relation. Now, let consider an arbitrary chordal decomposition into m chordal subgraphs $\{G_i\}_{i\in\{1,2,\dots,m\}}$. Since chordal graphs have no induced cycles of length greater than three, is implied that each chordal graph is also a perfect graph. Hence, for every chordal component G_i of our initial compatibility graph G, the following relation holds:

$$\alpha(G_i) = \theta(G_i) \qquad (4.1.2)$$

where $\alpha(G_i)$ and $\theta(G_i)$ are graph's G_i independence number and vertex clique cover number respectively. However the $\alpha(G_i)$ is also denoting the ND-bound of the chordal graph G_i. Therefore, the monogamy relation by the vertex decomposition into chordal subgraphs becomes:

$$\sum_{j=1}^{m}\theta(G_i) = \sum_{i=1}^{m}\alpha(G_i) \leq n \cdot R \tag{4.1.3}$$

This result is quite obvious, since each chordal subgraph can decomposed further into a set of cliques. This proves that the condition that the vertex clique cover number be equal to $n \cdot R$ is both necessary and sufficient for a compatibility graph to result in a contextual monogamy relation by the method outlined before.

□

4.2 KCBS inequalities monogamy relations

Let us remember the KCBS inequality again. It was originally introduced in order to test the "quantumness" of a single three – level system, and it basically constitutes a restrictive relation on the probabilities of pairwise mutually exclusive events. The KCBS inequality reads:

$$\sum_{i=0}^{4} p(A_i = 1) \leq 2 \tag{4.2.1}$$

Where the A_i , $i \in \mathbb{Z}_5$, represent five cyclically compatible observables which take binary values upon measurement. That means that each observable A_i, takes a value $a_i \in \{-1,1\}$ when measured, and also that is possible to determine the joint probabilities $p(a_i, a_{i+1})$ for every $i \in \mathbb{Z}_5$. Furthermore, the events $\{A_i = 1\}$ and $\{A_{i+1} = 1\}$ are mutually exclusive $\forall i \in \mathbb{Z}_5$, that is: $a_i a_{i+1} = 0$.

Now, we are going to formulate a specific scenario (Ramanathan et al 2012) in which two KCBS inequalities are involved, and then we are going to show the existence of a monogamy relation between them according to the outlined method above.

In order to do that, Consider two sets of cyclically compatible and exclusive measurements $\{A_i\}$ and $\{A'_i\}$ similar to the one we mentioned above, in a way that each set gives rise to a KCBS inequality. Furthermore, let assume that the triples $\{A_0, A'_0, A'_1\}$ and $\{A_3, A_4, A'_4\}$ are jointly measurable and mutually exclusive. Therefore, in addition to the joint probabilities $p(a_i, a_{i+1})$ and $p(a'_i, a'_{i+1})$ one can also determine the joint probabilities $p(a_0, a'_0, a'_1)$ and $p(a_3, a_4, a'_4)$. The compatibility graph that describes this setup is:

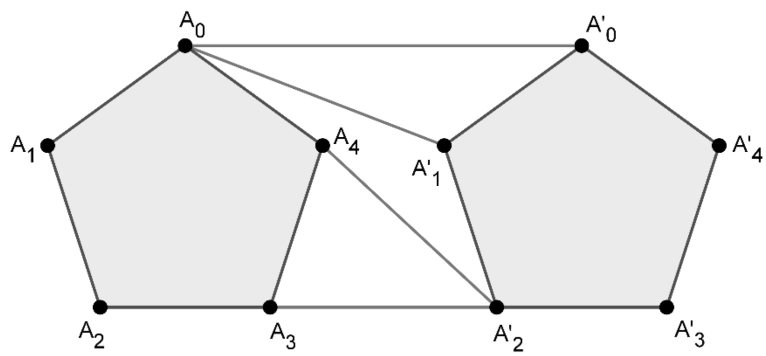


Fig. 4.2.1 Compatibility graph that includes two KCBS inequalities according to the scenario above.

Notice that we are able to perform a vertex decomposition on this graph such that each one of the induced subgraph components be a chordal graph. An example of such a decomposition is the following:

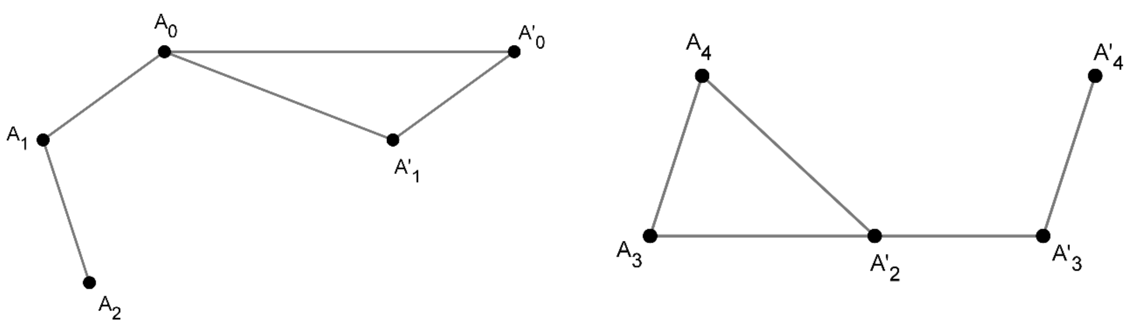


Fig. 4.2.2 The chordal subgraph decomposition according to the theory we introduced on the previous section

The independence of each component is 2, and thus the total ND-bound of the initial graph is 4 which the same as its NC-bound. Therefore we should have a monogamy relation between the two KCBS inequalities. Let explain this in more detail.

Due to the fact that Quantum theory satisfies the ND principle, we know that the probabilities $p(A_i = a_i)$ and $p(A'_i = a'_i)$ of the events $\{A_i = a_i\}$ and $\{A'_i = a'_i\}$ to occur should be the same independently of the measuring context. That allows us to set a fixed probability value for the occurrence of the events $\{A_i = 1\}$ and $\{A'_i = 1\}$. Let now assume that $p(A_0 = 1) = p$ and $p(A'_4 = 1) = q$. Since the events $\{A_0 = 1\}$, $\{A'_0 = 1\}$, $\{A'_1 = 1\}$ are disjoint, is implied that: $p(A_0 = 1) + p(A'_0 = 1) + p(A'_1 = 1) \leq 1$, and therefore,

$$p(A'_0 = 1) + p(A'_1 = 1) \leq 1 - p$$

In a similar way, the mutual exclusiveness of $\{A_3 = 1\}, \{A_4 = 1\}$, $\{A'_4 = 1\}$ implies that

$$p(A_3 = 1) + p(A_4 = 1) \leq 1 - q$$

We already know that the families of events $\{A_i = 1\}_i$ and $\{A'_i = 1\}_i$ are cyclically exclusive and therefore the following relations hold:

$$p(A_i = 1) + p(A_{i+1} = 1) \leq 1$$

$$p(A'_i = 1) + p(A'_{i+1} = 1) \leq 1$$

Now, by only assuming that the ND principle holds, we can conclude the following:

$$p(A_1 = 1) + p(A_2 = 1) \leq 1 \Longrightarrow$$
$$p(A_1 = 1) + p(A_2 = 1) + p(A_3 = 1) + p(A_4 = 1) \leq 2 - q \Longrightarrow$$
$$p(A_0 = 1) + p(A_1 = 1) + p(A_2 = 1) + p(A_3 = 1) + p(A_4 = 1) \leq 2 - q + p \Longrightarrow$$
$$\sum_{i=0}^{4} p(A_i = 1) \leq 2 - q + p$$

In the same way we can derive a similar inequality for the second family of observables:

$$\sum_{i=0}^{4} p(A_i = 1) \leq 2 - q + p$$

By summing up these two inequalities, we finally take our monogamy relation,

$$\sum_{i=1}^{5} p(A_i = 1) + \sum_{i=1}^{5} p(A'_i = 1) \leq 4$$

This relation is derived directly from the ND principle, and states that if someone tries to violate the KCBS inequality for one of the two observable families that we described above, then his measurements outcomes will be necessarily satisfying the KCBS inequality for the other observable family.

Now, we are going to present a setup, meaning a collection of observables, for which the above monogamous relation applies within the quantum theory. First, note that the observables for the optimal violation of KCBS inequality for a single qutrit system are rank-1 projectors spanning the three-dimensional real space. For our case, consider two families of observables $\{A_i\}$ and $\{A_i'\}$ on a four-dimensional space, where the set of projectors $\{A_i\}$ spans dimensions 1,2 and 3, and the set of projectors $\{A_i'\}$ spans dimensions 2,3 and 4. These projectors can be chosen accordingly, to obey the constraints of commutability and mutual exclusiveness as required be the KCBS compatibility graphs. A set of ten vectors in a 4-dimensional space that produces a set of projectors which corresponds to the measuring scenario (Fig.4.2.1) is given below (Ramanathan et al 2012):

$$|v_1\rangle = (1,0,0,0)^T,\ \ |v_2\rangle = (0,1,0,0)^T,\ \ |v_3\rangle = (\cos\theta\,, 0, \sin\theta\,, 0)^T,$$

$$|v_4\rangle = (\sin\varphi\sin\theta\,, \cos\varphi\,, -\sin\varphi\cos\theta\,, 0)^T,\ \ |v_5\rangle = (0, \sin\varphi\cos\theta\,, \cos\varphi\,, 0)^T$$

and

$$|v'_1\rangle = (0,0,0,1)^T,\ \ |v'_2\rangle = (0, \cos\alpha\,, \sin\alpha\,, 0)^T,\ \ ,$$

$$|v'_3\rangle = (0, \sin\beta\sin\alpha\,, -\sin\beta\cos\alpha\,, \cos\beta)^T,$$

$$|v'_4\rangle = (0, \sin\gamma\sin\delta\,, -\sin\gamma\cos\delta\,, \cos\gamma)^T,\ \ |v'_5\rangle = (0, \sin\gamma\cos\delta\,, \sin\gamma\sin\delta\,, 0)^T$$

where $\sin(\alpha-\delta) \neq 0$, $\cos(\alpha-\delta) \neq 0$ and $\tan\beta\tan\gamma\cos(\alpha-\delta) = -1$. The projectors $\{A_i\}$ and $\{A_i'\}$ are given by:

$$A_i = \frac{|v_i\rangle\langle v_i|}{\langle v_i|v_i\rangle}, \qquad A_i' = \frac{|v'_i\rangle\langle v'_i|}{\langle v'_i|v'_i\rangle}$$

These observables correspond exactly to the measurement configuration in (Fig.4.2.1).

4.3 Monogamy examples derived from Compatibility graphs

Now, we are going to study some simple examples on how to decompose a compatibility graph into chordal subgraphs. The following graphs correspond to systems where the observables behavior can be described via a set of KCBS type inequalities:

Example 1

A measurement configuration that gives rise to 2 KCBS inequalities

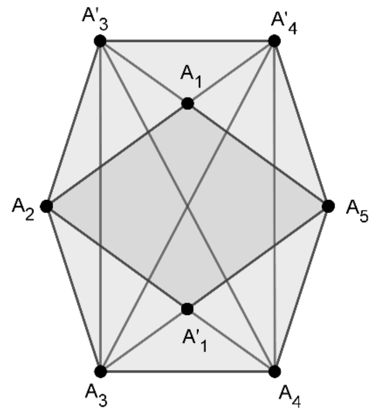


Fig. 4.3.3 Two overlapping KCBS compatibility graphs connected via exclusive relations

Notice that in this case we have two vertices that take part in both KCBS inequalities. Therefore in the chordal graph decomposition we will include them twice inside the components. Another way to resolve the issue of decomposition while having a graph with overlapping vertices, is two replace any overlapping vertex with a pair of compatible but not mutual exclusive vertices, where each of these two vertices has exactly the same neighbors with the one they replaced. Thus, the decomposition of this graph is the following two chordal subgraphs:

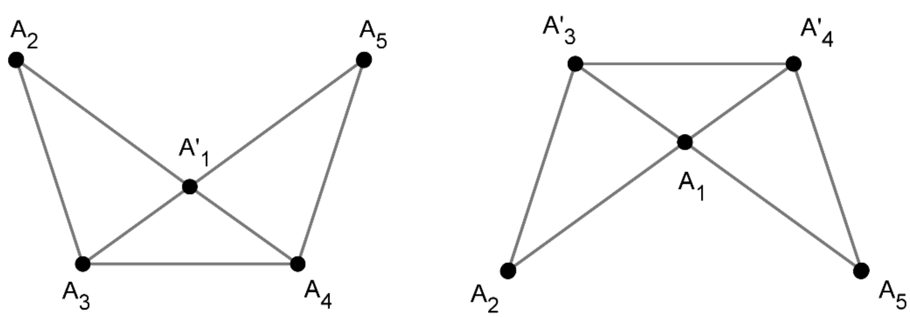


Fig. 4.3.2 The 2 induced chordal subgraph components

Since every edge of the initial graph denotes also mutual exclusiveness, we can compute the ND-bounds of these subgraphs by their independence number, which is 2 for both of them. That means,

$$p(A_2 = 1) + p(A_3 = 1) + p(A_4 = 1) + p(A_5 = 1) + p(A'_1 = 1) \underset{ND}{\leq} 2$$

$$p(A_2 = 1) + p(A_5 = 1) + p(A_1 = 1) + p(A'_3 = 1) + p(A'_4 = 1) \underset{ND}{\leq} 2$$

By summing them, we get the monogamy relation:

$$K(A_i) + K(A'_i) \underset{ND}{\leq} 4$$

The joint probability distributions for each chordal subgraph, by applying the method from proposition 1, are:

$$p(a_1, a_2, a'_3, a'_4, a_5) = \frac{p(a_1, a_2, a'_3)p(a_1, a'_3, a'_4)p(a_1, a'_4, a_5)}{p(a_1, a'_3)p(a_1, a'_4)}$$

$$p(a'_1, a_2, a_3, a_4, a_5) = \frac{p(a'_1, a_2, a_3)p(a'_1, a_3, a_4)p(a'_1, a_4, a_5)}{p(a'_1, a_3)p(a'_1, a_4)}$$

Example 2

A measurement configuration that gives rise to 2 KCBS inequalities with the following compatibility graph:

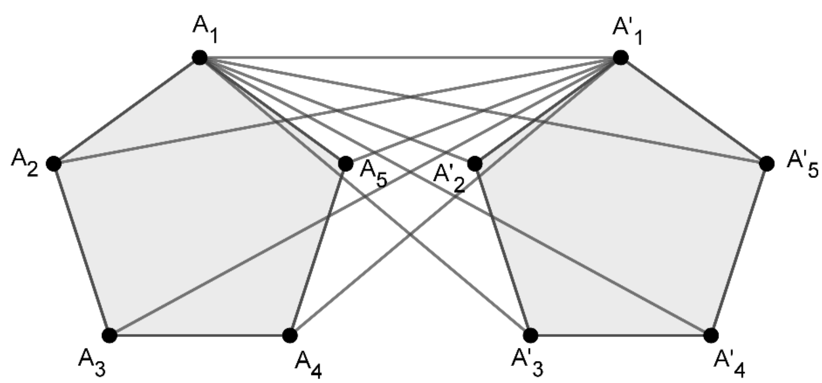


Fig. 4.3.3 two KCBS compatibility graphs connected via exclusive relations

By performing the chordal subgraph decomposition we obtain the following induced subgraphs:

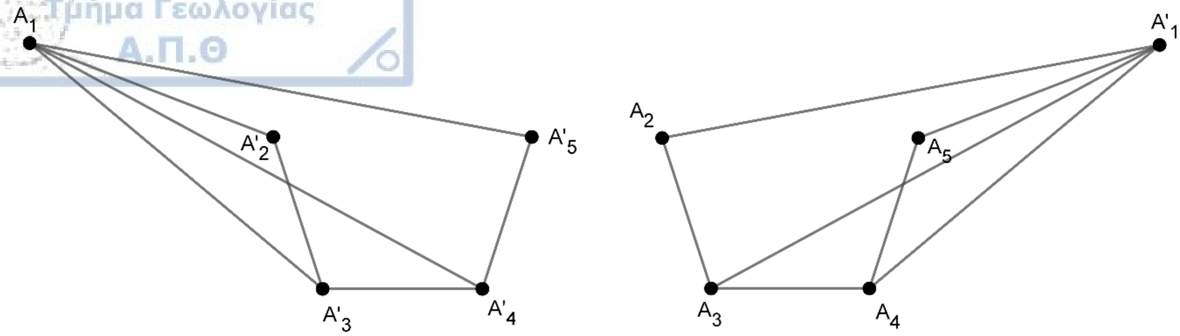


Fig. 4.3.4 The 2 induced chordal subgraph components of (Fig. 4.3.3)

Since the edges denote mutual exclusiveness we can conclude that the ND-bound of each subgraph is given by their independence number, which is 2 in both cases. Therefore, the ND-bound of the initial graph is 4 and thus we obtain a monogamy relation.

The joint probability distributions for each chordal subgraph, by applying the method from proposition 1, are:

$$p(a_1, a'_2, a'_3, a'_4, a'_5) = \frac{p(a_1, a'_2, a'_3)p(a_1, a'_3, a'_4)p(a_1, a'_4, a'_5)}{p(a_1, a'_3)p(a_1, a'_4)}$$

$$p(a'_1, a_2, a_3, a_4, a_5) = \frac{p(a'_1, a_2, a_3)p(a'_1, a_3, a_4)p(a'_1, a_4, a_5)}{p(a'_1, a_3)p(a'_1, a_4)}$$

Example 3

Let us study a case where three KCBS inequalities are involved. The measurement configuration is given the compatibility graph below, where the edges denote also exclusivity relations:

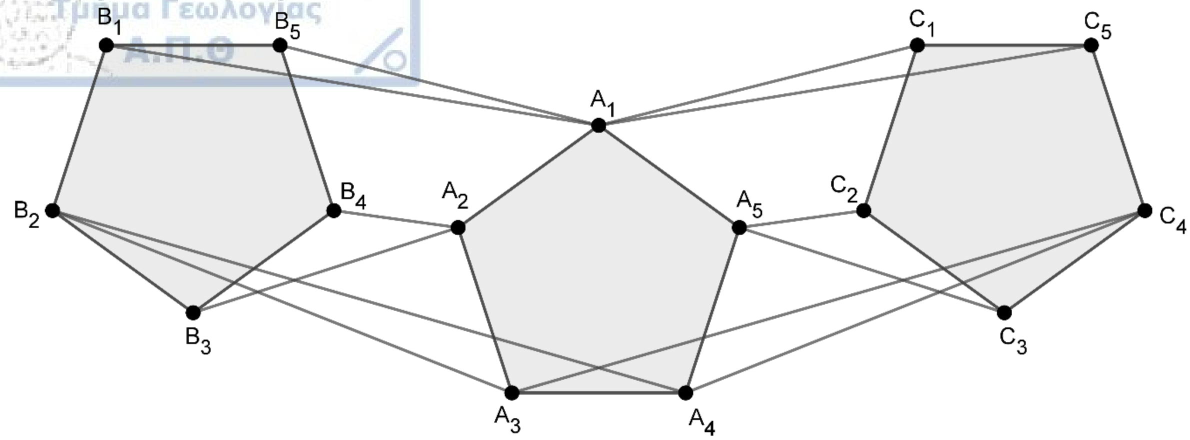


Fig. 4.3.5 The compatibility graph of a three KCBS inequalities scenario

We can perform a vertex decomposition of this graph into four induced chordal subgraphs:

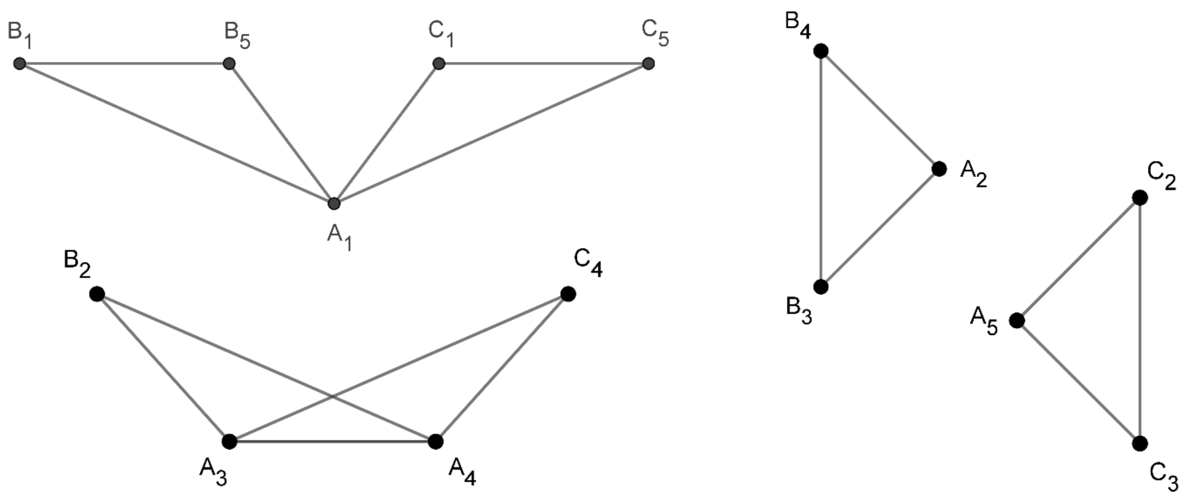


Fig. 4.3.6 The 4 induced chordal subgraph components of (Fig. 4.3.5)

The two chordal subgraph components on the left have independence number 2, while the other two on the right have independence number 1. That makes the total ND-bound of the initial graph 6 which is exactly the total NC-bound of the three KCBS inequalities. That indicates a monogamous relation between the three KCBS inequalities described by the initial compatibility graph.

The joint probability distributions for each chordal subgraph, by applying the method from proposition 1, are:

$$p(a_1, b_1, b_5, c_1, c_5) = \frac{p(a_1, b_1, b_5)p(a_1, c_1, c_6)}{p(a_1)}$$

$$p(a_3, a_4, b_2, c_4) = \frac{p(a_3, a_4, c_4)p(a_3, a_4, b_2)}{p(a_3, a_4)}$$

$$p(a_2, b_3, b_4) \quad , \quad p(a_5, c_2, c_3)$$

Example 4

Now, let see an example of a monogamous relation between a classic KCBS inequality, and a KCBS-type inequality with more than five observables. The first inequality is a classic KCBS inequality:

$$\sum_{i=1}^{5} p(A_i = 1) \leq 2$$

The second inequality scenario includes seven cyclic compatible $\{A'_i\}$ observables while the events $\{A'_i = 1\}$ and $\{A'_{i+1} = 1\}$, with respect to modulo 7 addition, are disjoint:

$$\sum_{i=1}^{7} p(A'_i = 1) \leq 3$$

Notice that the above inequality can indeed violated by quantum theory, since the corresponding exclusivity graph is a cycle with length seven, and thus a contextuality graph. Its compatibility graph is also a 7-cycle. The compatibility graph that describes our scenario is the following:

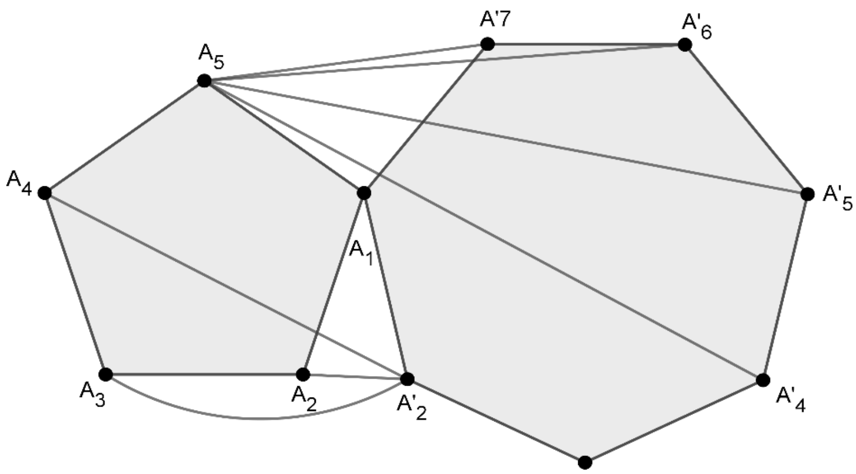


Fig. 4.3.7 Compatibility graph of a scenario involving a 5-KCBS and a 7-KCBS inequality.

Also notice that in our example, the vertex A_1 takes part in both inequalities, and thus we will include it twice in the vertex decomposition. Hence we can construct the following two induced chordal subgraphs:

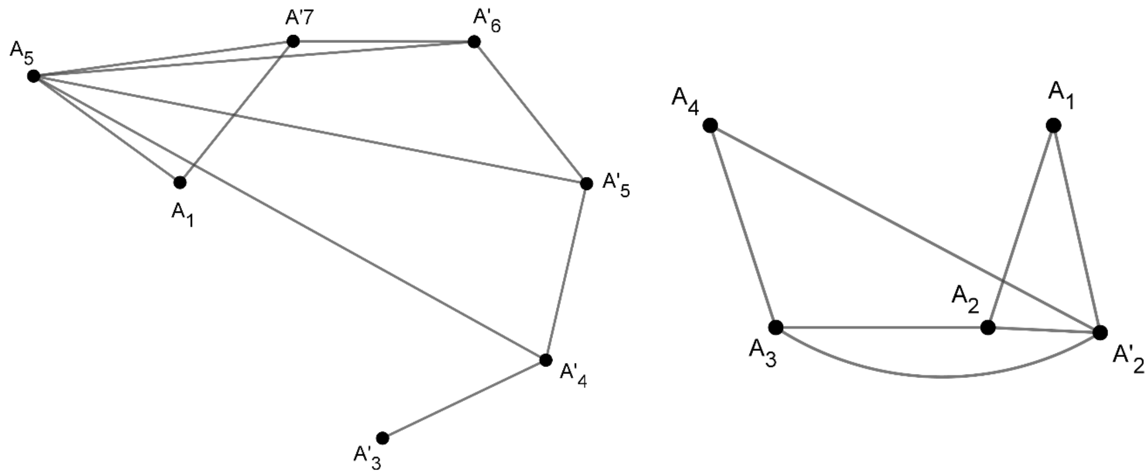


Fig. 4.3.8 The 2 induced chordal subgraph components of graph in (Fig. 4.3.7)

The left subgraph component has an independence number of 3, and the right subgraph component has an independence number of 2. Hence, the total ND-bound for the scenario is 5, which is exactly the sum of the corresponding inequalities NC-bounds. That ensures the monogamy relation.

The joint probability distributions for each chordal subgraph, by applying the method from proposition 1, are:

$$p(a_1, a'_7, a'_6, a'_5, a'_4, a'_3, a_5) =$$
$$= \frac{p(a_1, a'_7, a_5)p(a'_7, a'_6, a_5)p(a'_6, a'_5, a_5)p(a'_5, a'_4, a_5)p(a'_4, a'_3)}{p(a'_7, a_5)p(a'_6, a_5)p(a'_5, a_5)}$$

$$p(a_1, a_2, a_3, a_4, a'_2) = \frac{p(a_1, a_2, a'_2)p(a_2, a_3, a'_2)p(a_3, a_4, a'_2)}{p(a_2, a'_2)p(a_3, a'_2)}$$

Example 5

In this scenario, we will see the monogamy of a classical KCBS inequality with a KCBS-type with nine observables. Note that the corresponding Hilbert space of the system, in cases with more than five cyclical observables, needs to have dimensions greater than three. As in the previous example, a KCBS scenario with nine cyclical compatible observables induces a contextuality exclusivity graph, and thus the corresponding inequality can be violated by the Quantum theory. This scenario is described via this compatibility graph:

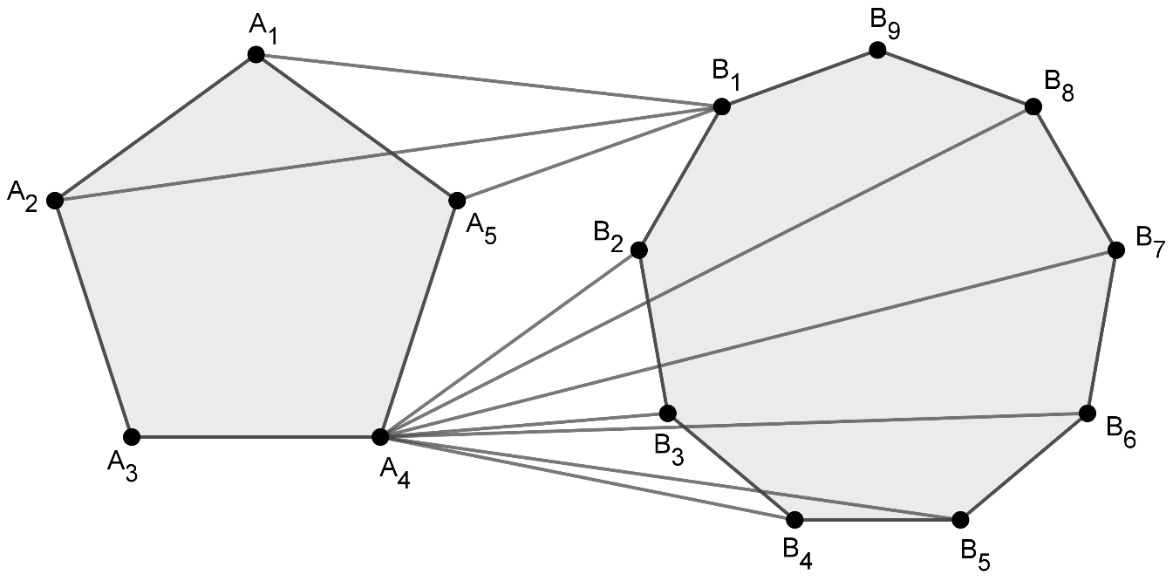


Fig. 4.3.9 Compatibility graph of a scenario involving a 5-KCBS and a 9-KCBS inequality.

By performing a vertex decomposition with the outlined method we obtain the following two induced chordal subgraphs:

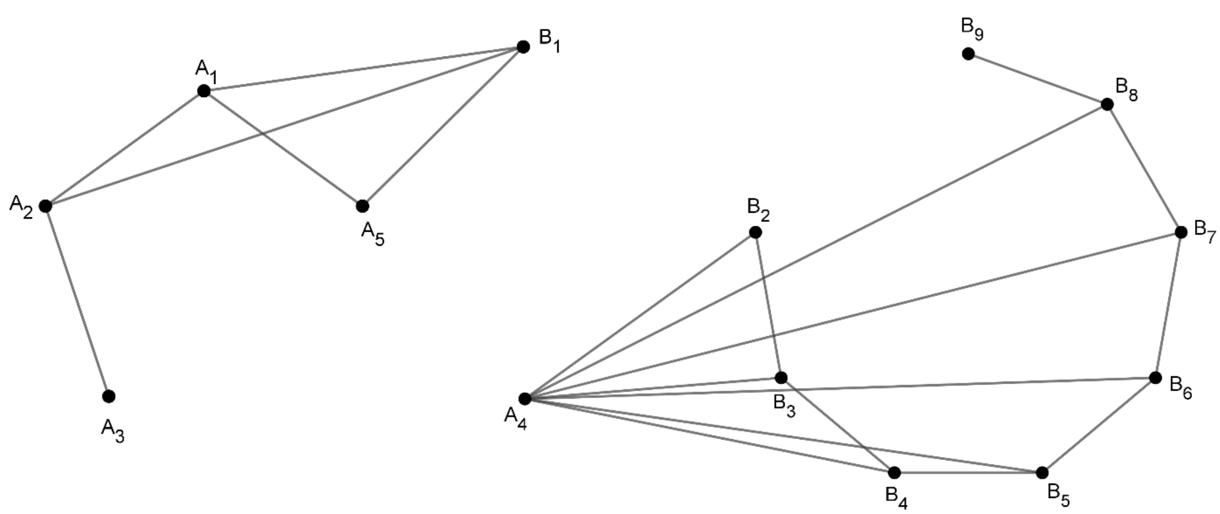


Fig. 4.3.10 The 2 induced chordal subgraph components of graph in (Fig. 4.3.9)

The ND-bound of these subgraphs are 2 for the left, and 4 for the right one. The total ND-bound of the compatibility graph is 6 which is the same as its NC-bound. Therefore, a monogamy relation holds.

The joint probability distributions for each chordal subgraph, by applying the method from proposition 1, are:

$$p(a_1, a_2, a_3, a_4, a_5, b_1) = \frac{p(a_1, a_5, b_1)p(a_1, a_2, b_1)p(a_2, a_3)}{p(a_1, b_1)}$$

$$p(a_4, b_2, b_3, b_4, b_5, b_6, b_7, b_8, b_9) =$$

$$= \frac{p(b_2, b_3, a_4)p(b_3, b_4, a_4)p(b_4, b_5, a_4)p(b_5, b_6, a_4)p(b_6, b_7, a_4)p(b_7, b_8, a_4)p(b_8, b_9)}{p(b_3, a_4)p(b_4, a_4)p(b_5, a_4)p(b_6, a_4)p(b_7, a_4)}$$

4.3.1 Remark

If A, B and C are three pairwise compatible observables and $\hat{A}$, $\hat{B}$, $\hat{C}$ are their corresponding operators, then the joint probability distribution when performing a measurement with an initial state $|\psi\rangle$, is given by: $p(a, b, c) = \langle\psi|P_a P_b P_c|\psi\rangle$, where P_a, P_b, P_c are the projector operators of the eigenspaces of $\hat{A}$, $\hat{B}$ and $\hat{C}$ that correspond to outcomes a, b and c respectively.

4.4 CHSH monogamy

In this section we are going to show that a monogamy relation, similar to the ones we study before, is underlying any Bell scenario. More specifically we are going to show that the quantum correlations between three qubit systems, which is the simplest case, exhibit a monogamous behavior. This proposition is analogous to the monogamy of entanglement (Coffman et al, 2000), however, in our approach we will make use of the system's compatibility graph and the method illustrated in the section ….. in order to obtain a monogamy relation of two CHSH inequalities.

Let Alice, Bob and Charlie be three observers, with each one of them performing measurements on a qubit-system with two possible settings. Bob and Charlie simultaneously try to violate a Bell-CHSH inequality with Alice using two measurement settings each. Therefore, our scenario consists of six observables and two CHSH sub-scenarios: one CHSH inequality that describes the correlations in the Alice-Bob system, and another one for the Alice-Charlie system. If we denote the measurements performed by Alice as A_1 and A_2, by Bob as B_1 and B_2, and by Charlie as C_1 and C_2, the spatial separation guarantees that any set of observables $\{A_i, B_j\}$, $\{A_i, C_k\}$, or $\{B_j, C_k\}$ corresponds to compatible measurements, though not mutually exclusive, while the measurement pairs $\{A_1, A_2\}$, $\{B_1, B_2\}$ and $\{B_1, B_2\}$ cannot be jointly performed. Additionally, we will consider that the outcome of a measurement will be either 1 or -1. The compatibility graph that describes the above scenario is the following:

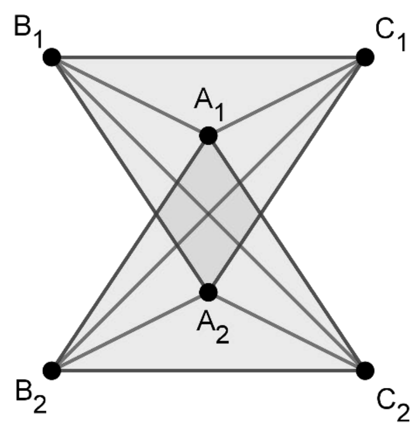


Fig. 4.4.1 Compatibility graph of measuring three qubit subsystems. Here the edges do not denote mutual exclusiveness

Notice that contrary to the KCBS cases, the edges in this compatibility graph do not imply mutual exclusiveness between the corresponding events. This compatibility graph gives rise to two separate CHSH tests, for which the following inequalities hold:

$$\beta(A_1, A_2, B_1, B_2) = P(1,1|A_1, B_1) + P(-1,-1|A_1, B_1) + P(1,1|A_1, B_2) + P(-1,-1|A_1, B_2) + P(1,1|A_2, B_1) + P(-1,-1|A_2, B_1) + P(1,-1|A_2, B_2) + P(-1,1|A_2, B_2) \underset{LHV}{\leq} 3 \tag{4.4.1a}$$

$$\beta(A_1, A_2, C_1, C_2) = P(1,1|A_1, C_1) + P(-1,-1|A_1, C_1) + P(1,1|A_1, C_2) + P(-1,-1|A_1, C_2) + P(1,1|A_2, C_1) + P(-1,-1|A_2, C_1) + P(1,-1|A_2, C_2) + P(-1,1|A_2, C_2) \underset{LHV}{\leq} 3 \tag{4.4.1b}$$

By using the method outlined in the section …. We can decompose the scenario's compatibility graph into two isomorphic induced chordal subgraphs G_1 and G_2:

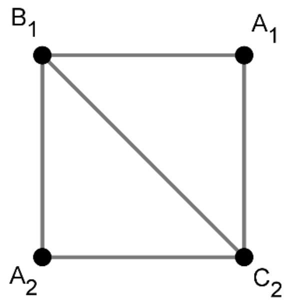


Fig. 4.4.3a Induced chordal subgraph G1

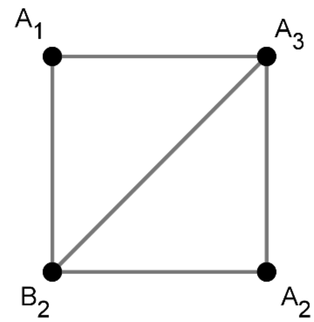


Fig. 4.4.3b Induced chordal subgraph G2

Each of these subgraphs induces a joint probability distribution, and thus any associated inequality that come of these graphs cannot be violated by the Quantum theory. In order to check if the derivation of a monogamous relation is achievable, we need to compute the NC-bounds from the appropriate corresponding exclusivity graphs. By "appropriate" we mean that the choice of events used for the generation of the two exclusivity graphs, have to be the same as the ones appearing in the original CHSH inequalities.

Hence, the exclusivity graphs of the chordal subgraph components for the initial collection of events are:

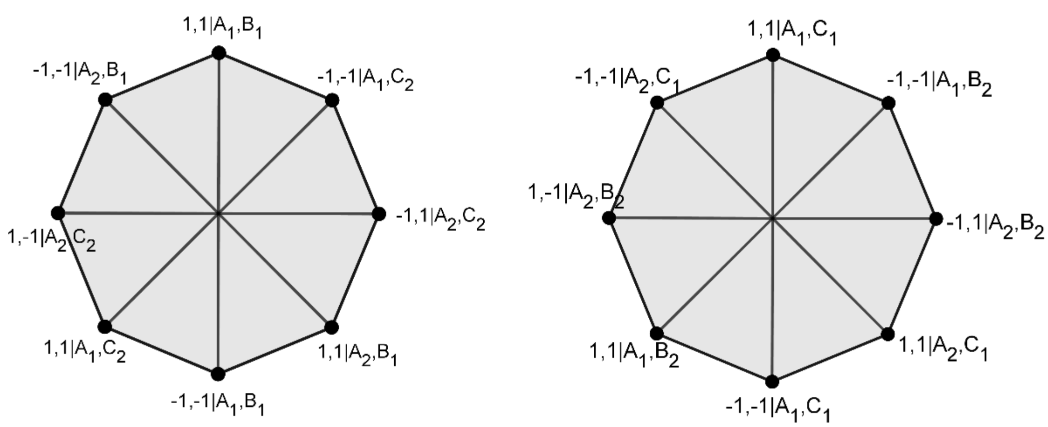


Fig. 4.4.3 Exclusivity graphs corresponding to events from measurements from the chordal subgraphs

As we can see, the exclusivity graphs are both isomorphic to the original CHSH exclusivity graph. Their independence number, and therefore their NC-bound, is equal to 3. That, gives rise to the following inequalities:

$$\begin{gathered}P(1,1|A_1,B_1)+P(-1,-1|A_1,B_1)+P(1,1|A_2,B_1)+P(-1,-1|A_2,B_1)+\\P(1,1|A_1,C_2)+P(-1,-1|A_1,C_2)+P(1,-1|A_2,C_2)\\+P(-1,1|A_2,C_2)\underset{NHV}{\leq}3\end{gathered} \tag{4.4.2a}$$

$$\begin{gathered}P(1,1|A_1,C_1)+P(-1,-1|A_1,C_1)+P(1,1|A_2,C_1)+P(-1,-1|A_2,C_1)+\\P(1,1|A_1,B_2)+P(-1,-1|A_1,B_2)+P(1,-1|A_2,B_2)\\+P(-1,1|A_2,B_2)\underset{NHV}{\leq}3\end{gathered} \tag{4.4.2b}$$

However, unlike the original case of CHSH, here the compatibility graphs allows us to construct the following two joint probability distributions, for G1 and G2 respectively:

$$p_1(a_1,a_2,b_1,c_2)=\frac{p(a_1,b_1,c_2)p(a_2,b_1,c_2)}{p(b_1,c_2)} \tag{4.4.3a}$$

$$p_2(a_1,a_2,b_2,c_1)=\frac{p(a_1,b_2,c_1)p(a_2,b_2,c_1)}{p(b_2,c_1)} \tag{4.4.3b}$$

Also, the no-signaling principle ensures us that any marginal probability distribution we can measure, is the same independently from the joint distribution it came from. This allows us to write the probabilities appearing in the inequalities (4.4.2a) and (4.4.2b) as marginals of the joint distributions $p_1(a_1,a_2,b_1,c_2)$ and $p_2(a_1,a_2,b_2,c_1)$ respectively. By replacing the events of the inequalities with the corresponding sum of disjoint elementary events that take art in p_1 and p_2, one can easily see that the NC-bound of these inequalities is equal to their ND-bound. By summing up these two non-contextual inequalities we obtain a third non-contextual inequality with an ND-bound of 6:

$$\begin{gathered}P(1,1|A_1,B_1)+P(-1,-1|A_1,B_1)+P(1,1|A_2,B_1)+P(-1,-1|A_2,B_1)+\\P(1,1|A_1,C_2)+P(-1,-1|A_1,C_2)+P(1,-1|A_2,C_2)+P(-1,1|A_2,C_2)+\\P(1,1|A_1,C_1)+P(-1,-1|A_1,C_1)+P(1,1|A_2,C_1)+P(-1,-1|A_2,C_1)+\\P(1,1|A_1,B_2)+P(-1,-1|A_1,B_2)+P(1,-1|A_2,B_2)+P(-1,1|A_2,B_2)\underset{ND}{\leq}6\end{gathered} \tag{4.4.4}$$

However, notice that the left-hand side of the inequality is the sum of the two initial CHSH expressions:

$$\beta(A_1,A_2,B_1,B_2)+\beta(A_1,A_2,C_1,C_2)\underset{ND}{\leq}6 \tag{4.4.5}$$

And this is exactly the expression that establishes the monogamous relation between the two CHSH inequalities, as only one of them may be violated. If both of them ought to be violated, then there would also be also a violation of the bound acquired from the No-Disturbance principle, and this is impossible in the context of Quantum theory.

4.5 Monogamy relation between Contextuality and Nonlocality

Finally we are going to show that there is monogamy relation between the KCBS and CHSH inequalities, on a paired qutrit-qubit system [Kurzyński, 2014]. In order to prove that we need to consider the following scenario: Alice (observer A) and Bob (observer B) share pairs of correlated systems, and are able to perform binary measurements on these systems. Let these systems be qutrits for Alice and qubits for Bob. Alice is able perform five measurements $\{A_1, \dots, A_5\}$ on her system, from which, every two consecutive observables A_i, A_{i+1}, with respect to the sum modulo 5, are compatible with each other. On the other hand, Bob is able to perform two measurements $\{B_1, B_2\}$ on his system, which are incompatible with each other, but at the same time each B_j is compatible with all the Alice's observables A_i. Also, each of Bob's and Alice's measurements have only two possible outcomes: $+1$ or -1. The compatibility relations among the seven measurements are illustrated in the figure below [Kurzyński, 2014]:

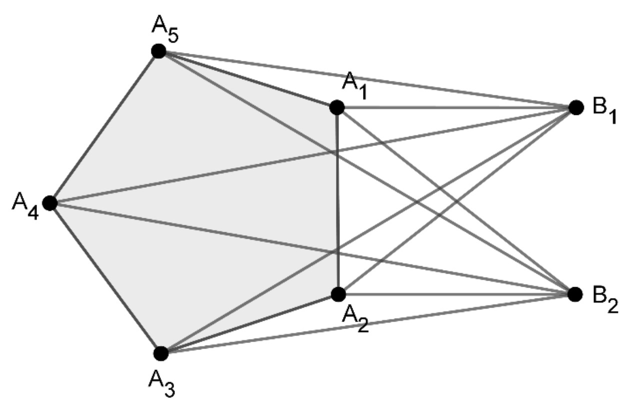


Fig. 4.5.1 The compatibility graph of the paired qutrit-qubit scenario. The edges (A_i, A_{i+1}) also denote mutual exclusiveness, while the edges (A_i, B_j) denote only compatibility

For each pair of systems that Alice shares with Bob, she randomly chooses to measure two compatible observables A_i and A_{i+1}, while Bob chooses to measure only one of his incompatible observables. After repeating the experiment many times, Alice and Bob can evaluate the following correlations, that is the mean values of the products of outcomes:

$$\langle A_i A_{i+1} \rangle, \langle A_i B_j \rangle, \langle A_i A_{i+1} B_j \rangle \tag{4.5.1}$$

Where $i \in \mathbb{Z}_5$ and $j = 1,2$. These correlations can be used in used in two different tests. The first one is a test of the KCBS non-contextuality inequality on Alice's qutrit system, i.e.,

$$\kappa_A = \langle A_1A_2\rangle + \langle A_2A_3\rangle + \langle A_3A_4\rangle + \langle A_4A_5\rangle + \langle A_5A_1\rangle \underset{NCHV}{\geq} -3 \tag{4.5.2}$$

The second one is a test of CHSH Bell inequality between Alice's and Bob's subsystems, i.e.,

$$\beta_{AB} = \langle A_{i+1}B_1\rangle + \langle A_{i+1}B_2\rangle + \langle A_{i-1}B_1\rangle - \langle A_{i-1}B_2\rangle \underset{LHV}{\geq} -2 \tag{4.5.3}$$

Where A_{i+1} and A_{i-1} can be any two incompatible measurements from Alice's set.

The violation of either the KCBS or the CHSH inequality implies that the corresponding correlations cannot be described by a non-contextual or a local hidden variable model respectively. On the other hand, the satisfaction of these inequalities would make the existence of a hidden variable theory (HV) a possible scenario. Also, since the No Disturbance (ND) principle is a general condition satisfied by all the current physical theories, is implied that this particular scenario must have an ND-bound that imposes a restriction upon the possible outcomes that we can acquire in the context of Quantum theory. As we have seen, we can consider that Bell's non-locality constitutes a special case of contextuality, and as an immediate result we can consider that Bell type inequalities are also non-contextuality inequalities [Abramsky et al, 2011]. That, allows us to subtract or take the sum of both inequalities in order to produce a new non-contextuality inequality. Taking the sum of the KCBS and CHSH inequalities associating with the system that we have described above, we get:

$$\begin{aligned} C^{(i)} = \langle A_1A_2\rangle + \langle A_2A_3\rangle + \langle A_3A_4\rangle + \langle A_4A_5\rangle + \langle A_5A_1\rangle + \langle A_{i+1}B_1\rangle \\ + \langle A_{i+1}B_2\rangle + \langle A_{i-1}B_1\rangle - \langle A_{i-1}B_2\rangle \underset{NCHV}{\geq} -5 \end{aligned} \tag{4.5.4}$$

However, the ND-bound of the inequalities sum is not given by summing up their individual bounds. We can find this bound, by finding vertex subsets of the scenario's compatibility graph, which induce non-contextual graphs, meaning graphs that correspond

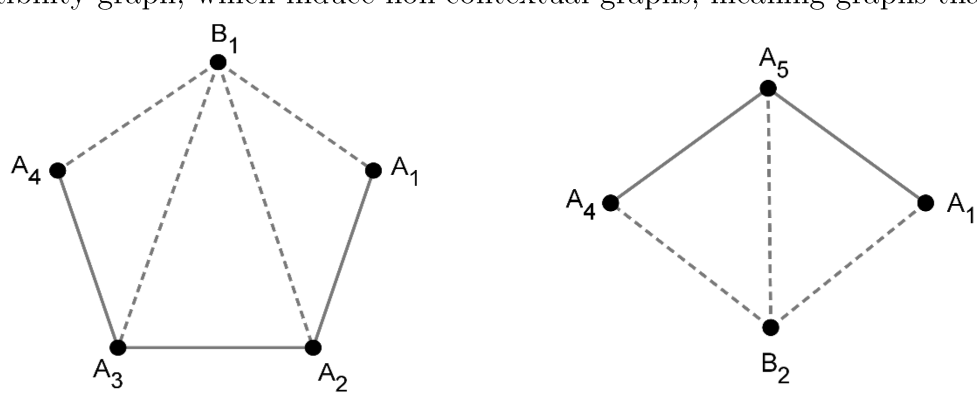


Fig. 4.5.2 Decomposition into induced chordal subgraphs

to inequalities inviolable by an ND theory. As we have seen from proposition (4.1.4), this can be achieved by finding chordal subgraph components of the initial graph. Let see an example of such a decomposition:

Where the continuous-line edges denote mutual exclusiveness additional to compatibility, while the dashed-line edges denote only the compatibility relation.

Now, according to the decomposition above, we can split the terms of the inequality (4.5.4) into two new components $C_1^{(i)}$ and $C_2^{(i)}$, such that:

$$C_1^{(i)} + C_2^{(i)} \underset{NCHV}{\geq} -5 \tag{4.5.5}$$

Where

$$C_1^{(i)} = \langle A_{i+1}B_1\rangle + \langle A_{i+1}A_{i+2}\rangle + \langle A_{i+2}A_{i-2}\rangle + \langle A_{i-2}A_{i-1}\rangle + \langle A_{i-1}B_1\rangle \tag{4.5.6a}$$

$$C_2^{(i)} = \langle A_{i+1}A_i\rangle + \langle A_{i-1}A_i\rangle + \langle A_{i+1}B_2\rangle - \langle A_{i-1}B_2\rangle \tag{4.5.6b}$$

Also, note that the expressions (4.5.6a) and (4.5.6b) have the same form as the KCBS and CHSH expressions respectively. Due to the fact that these expressions are structurally the same as the aforementioned non-contextual inequalities, we can derive their corresponding non-contextual bounds in a similar way to the one we used for the KCBS and CHSH scenarios. One can easily see, that the non-contextual bounds end up to be the same as the ones in the test inequalities. However, unlike the original inequalities, in these cases, the compatibility graphs describing the corresponding scenarios are chordal graphs and thus non-contextual graphs, meaning that the non-contextual bound is also the bound provided by acceptance of the ND principle. Therefore, the bounds of $C_1^{(i)}$ and $C_2^{(i)}$ for any theory satisfying the ND principle are

$$C_1^{(i)} \underset{ND}{\geq} -3 \tag{4.5.7a}$$

$$C_2^{(i)} \underset{ND}{\geq} -2 \tag{4.5.7b}$$

This came from the fact that we are able to construct a joint probability distribution for all the measurement statistics involved in $C_1^{(i)}$ and $C_2^{(i)}$. This can be achieved, by applying the method illustrated in the previous section. Following the constructive proof of (4.1.4), one can derive the following joint probability distributions:

For $C_1^{(i)}$,

$$p(a_{i+1}, a_{i+2}, a_{i-1}, a_{i-2}, b_1) = \frac{p(a_{i+1}, a_{i+2}, b_1)p(a_{i+1}, a_{i-2}, b_1)p(a_{i-1}, a_{i+2}, b_1)}{p(a_{i+2}, b_1)p(a_{i-2}, b_1)} \quad (4.5.8)$$

And similarly for $C_2^{(i)}$,

$$p(a_{i-1}, a_i, a_{i+1}, b_2) = \frac{p(a_i, a_{i-1}, b_2)p(a_i, a_{i+1}, b_2)}{p(a_i, b_2)} \quad (4.5.9)$$

Where we denoted $p(a_i) = p(A_i = a_i)$ for simplicity. Note, that the above joint distributions also recover all the measurable marginal distributions. For example, one may calculate the marginal $p(a_{i-1}, a_i)$ from $p(a_{i-1}, a_i, a_{i+1}, b_2)$ in the following way:

$$\sum_{a_{i+1}, b_2} p(a_{i-1}, a_i, a_{i+1}, b_2) = \sum_{b_2} \left(\sum_{a_{i+1}} \frac{p(a_i, a_{i-1}, b_2)p(a_i, a_{i+1}, b_2)}{p(a_i, b_2)} \right) =$$

$$\sum_{b_2} p(a_i, a_{i-1}, b_2) = p(a_{i-1}, a_i)$$

Of course, we can also calculate the probability $p(a_{i+1}, a_i)$ as well:

$$\sum_{a_{i-1}, b_2} p(a_{i-1}, a_i, a_{i+1}, b_2) = \sum_{b_2} \left(\sum_{a_{i-1}} \frac{p(a_i, a_{i-1}, b_2)p(a_i, a_{i+1}, b_2)}{p(a_i, b_2)} \right) =$$

$$\sum_{b_2} p(a_i, a_{i+1}, b_2) = p(a_{i+1}, a_i)$$

Notice that in both derivations we assumed that

$$\sum_{a_{i+1}} p(a_i, a_{i+1}, b_2) = \sum_{a_{i-1}} p(a_i, a_{i-1}, b_2) = p(a_i, b_2) \quad (4.5.10)$$

which is exactly the ND principle. Note that since these probabilities are defined within ND theories, we can recover any measurable marginal that is compliant with the ND principle.

The existence of a joint probability distribution for $C_1^{(i)}$ and $C_2^{(i)}$ guarantees that the inequalities (4.5.7a) and (4.5.7b) are always satisfied within an ND theory, and thus their sum is also bounded from below by -5.

$$C_1^{(i)} + C_2^{(i)} \underset{ND}{\geq} -5 \quad (4.5.11)$$

This implies that in any ND theory there is a monogamy relation between the KCBS and CHSH inequalities, i.e. at most one of them can be violated:

$$\kappa_A + \beta_{AB} \underset{ND}{\geq} -5 \tag{4.5.12}$$

5 Conclusions

In this thesis we presented and analyzed the concepts of non-locality and contextuality and we studied the monogamous relations that may appear between different non-locality or non-contextuality testing inequalities. We analyzed the Bell-Kochen-Specker theorem, and showed why a hidden variable model cannot describe effectively the quantum correlations. We also presented the basic non-contextuality and locality test inequalities, and approached the concept of contextuality from a graph-theoretical point of view. We classified the kinds of compatibility and exclusivity graphs into those who induce a non-contextual model and to those who do not. Then, we show a method illustrated by Ramanathan et al, for the derivation of a monogamy relation between different inequalities, and finally, we applied that method, and we constructed, or presented, some interesting examples of contextual monogamous relations.

5.1 Added value – Interesting Applications

The detection of a monogamous relation between two or more non-contextual inequalities, provides us with knowledge about the restrictions that quantum theory imposes to the transmissions of quantum signals. Very shortly we will mention two possible applications that point out the added value of the theoretical structure we presented.

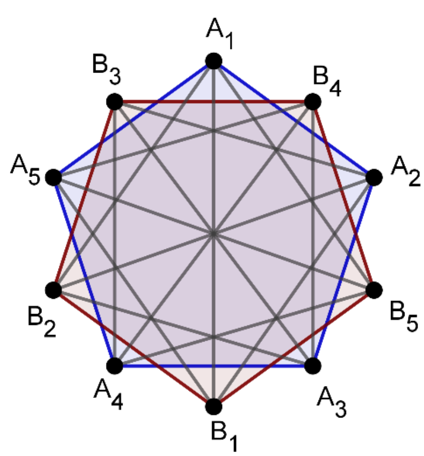
Qubit networks

As we have seen in section 4.4, the quantum correlations in a system of many paired qubits are bounded by a monogamous relation. That is a fundamental restriction which is imposed by quantum theory, and if we aim to create functional qubit networks [Tran et al, 2018], we need to take account of it. Quantum networks are not only essential for quantum communications [Kimble, 2008], but for quantum computation as well [Caleffi et al, 2018]. The qubit-type systems are the most basic quantum systems we employ in order to construct quantum processors. By linking multiple quantum processors we could create quantum computing clusters and therefore more computing potential.

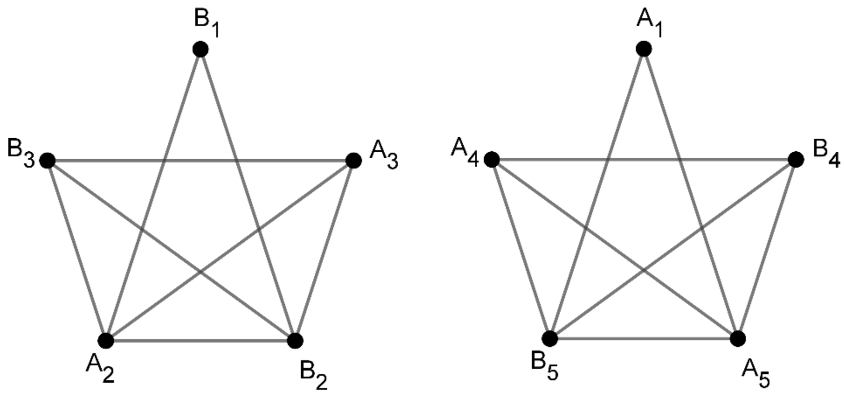
QKD

An interesting application that make use of the contextuality monogamies relations is the quantum key distribution (QKD). The most usual QKD protocol is the BB84 [Bennett, Brassard, 1984] protocol, where one party prepares a state and transmits it to the other party who performs suitable measurements to generate a key. However, it is possible to devise a QKD protocol between two different parties, by utilizing the KCBS scenario of contextuality as a resource [Singh et al, 2017]. We are now going to swiftly present the basic idea behind this model's security.

This QKD protocol [Singh 2017], use the KCBS monogamy relation in order to ensure a secure transmission. Consider two separated parties, Alice and Bob, that want to share a secret key securely, and an eavesdropper Eve who tries to obtain information about the correlation between Alice and Bob and the associated key. The compatibility graph that describes this scenario, is the following:



In this graph, the blue pentagon $\{A_i\}$ denotes the KCBS sub-scenario between Alice and Bob, while the red pentagon $\{B_i\}$ denotes the KCBS sub-scenario between Alice and Eve. According to the theory we have presented, we can try to decompose this graph into two induced chordal subgraphs with total ND-bound equal to the initials graph NC-bound. Therefore we obtain:



The total ND-bound of these two subgraphs is 4 which is exactly the total NC-bound of the scenarios compatibility graph. Hence we obtain a monogamous relation between the correlations distributed to the pair Alice – Bob and Alice – Eve. This fact is the basis for a security analysis that will inform us about the existence of an eavesdropper and whether or not the key distribution is successful.

5.2 Our contribution

By studying the related scientific publications, we worked on presenting a summary of the most important theorems on quantum contextuality and contextuality monogamy. Our original contribution is summarized to the following: We constructed the examples 3, 4 and 5 in the section 4.3, showing some interesting cases for the figures (Fig.4.2.2), (Fig.4.5.2),(Fig.3.2.2) and (3.2.6) according to the related theory, we wrote the related analysis for the CHSH's monogamy case in the section 4.4 (the decomposition was taken from [Ramanathan 2012]), and we formulated the proposition (4.1.3).

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