### Contextuality and Temporal Quantum Correlations





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- Motivation: Contextuality and sequential measurements
- Simulating temporal quantum correlations
- Tsirelson bounds for sequential measurements
- Structure of temporal correlations

# Contextuality and sequential measurements



# The Kochen-Specker theorem



Quantum mechanics cannot be explained by non-contextual hidden variable models.

What does non-contextuality mean?

### Compatibility and Noncontextuality

#### Compatibility

Two measurements A and B are compatible  $(A \sim B)$  if they can be measured simultaneously or in any order without disturbance.

#### Non-contextuality

Assume that  $A \sim B$  and  $A \sim C$ . A theory is non-contextual, if it assigns to A a value v(A) independently whether B or C is measured jointly with A.

#### KS Theorem

Such models are in conflict with quantum theory

### The Peres Mermin square

Consider a four level system (two qubits) and the observables:

$$\begin{array}{ll} A = \sigma_z \otimes \mathbbm{1}, & B = \mathbbm{1} \otimes \sigma_z, & C = \sigma_z \otimes \sigma_z, \\ a = \mathbbm{1} \otimes \sigma_x, & b = \sigma_x \otimes \mathbbm{1}, & c = \sigma_x \otimes \sigma_x, \\ \alpha = \sigma_z \otimes \sigma_x, & \beta = \sigma_x \otimes \sigma_z, & \gamma = \sigma_y \otimes \sigma_y. \end{array}$$

- The observables in each row (*R<sub>i</sub>*) and column (*C<sub>j</sub>*) commute and are compatible.
- If we assign to each of them a value  $v = \pm 1$  independently of the row or column, we have

$$\prod_{i=1}^{3} R_i C_i = +1$$

• In QM: 
$$C_3 = Cc\gamma = -1$$
, hence  $\prod_{i=1}^3 R_i C_i = -1$ .

A. Peres, PLA 151, 107 (1990); D. Mermin, PRL 65, 3373 (1990).

### A testable inequality

#### Question

Can we translate this into an experimentally testable inequality?

#### Answer

Consider sequences of measurements. Then, for non-contextual models

$$\begin{aligned} \langle \mathcal{X}_{\mathrm{MP}} \rangle &= & \langle A_1 B_2 C_3 \rangle + \langle a_1 b_2 c_3 \rangle + \langle \alpha_1 \beta_2 \gamma_3 \rangle \\ &+ \langle A_1 a_2 \alpha_3 \rangle + \langle B_1 b_2 \beta_3 \rangle - \langle C_1 c_2 \gamma_3 \rangle \\ &= \langle R_1 \rangle + \langle R_2 \rangle + \langle R_3 \rangle + \langle C_1 \rangle + \langle C_2 \rangle - \langle C_3 \rangle \leq 4. \end{aligned}$$

Here,  $\langle A_1 B_2 C_3 \rangle$  means the product of the values, when the sequence  $A_1 B_2 C_3$  is measured on a single instance of a state. In QM:

#### $\langle \mathcal{X}_{\mathrm{MP}} angle = 6$

for any quantum state (in contrast to a Bell inequality violation).

A. Cabello, PRL 101, 210401 (2008).

### Sequential measurements motivate noncontextuality

Assume that  $A \sim B$  and  $A \sim C$ . A theory is non-contextual, if it assigns to A a value v(A) independently whether B or C is measured jointly with A.

#### Bell

"... there is no a priori reason to believe that the results for  $|\phi_3\rangle\langle\phi_3|$  should be the same. The result of an observation may reasonably depend not only on the state of the system (including hidden variables), but also on the complete disposition of the apparatus"

J.S. Bell, Rev. Mod. Phys. 38 227 (1966).

#### Peres

"Suppose that we measure A first and only a later time decide whether to measure B or C or none of them. How can the outcome of the measurement A depend on this future decision?"

A. Peres, A. Ron, in "Microphysical Reality and Quantum Formalism" Kluwer, 1998.

### Other sequential inequalities



### Beyond the Peres Mermin inequality

**CHSH** Inequality

$$\langle A_1 \otimes B_1 \rangle + \langle A_1 \otimes B_2 \rangle + \langle A_2 \otimes B_1 \rangle - \langle A_2 \otimes B_2 \rangle \leq 2$$

This can also be seen as a temporal inequality.

Klyachko (KCBS) Inequality

 $\langle AB 
angle_{seq} + \langle BC 
angle_{seq} + \langle CD 
angle_{seq} + \langle DE 
angle_{seq} - \langle DA 
angle_{seq} \leq 3$ 

This can be violated in a three-dimensional system.

Leggett-Garg Inequality

 $\langle M(t_1)M(t_2)
angle_{seq}+\langle M(t_1)M(t_3)
angle_{seq}-\langle M(t_1)M(t_2)
angle_{seq}\leq 1$ 

This holds for macrorealistic models.

# Yu and Oh

#### Question

What is the simplest proof of contextuality?

#### The YO construction

- Take 13 vectors |v<sub>i</sub>⟩ in d=3 such that connected vectors are orthogonal.
- Take the observables

 $A_i = \mathbb{1} - 2 |v_i\rangle \langle v_i|$ 



Then, for non-contextual theories we have:

$$4\sum_{i\in V} \langle A_i\rangle - \sum_{(i,j)\in E} \left( \langle A_iA_j\rangle + \langle A_jA_i\rangle \right) \stackrel{\mathsf{NCHV}}{\leq} 32 \stackrel{\mathsf{QM}}{\leq} 32 + \frac{4}{3},$$

S. Yu, C.H. Oh, PRL 108, 030402 (2012), for an improvement see: M. Kleinmann et al., PRL 109, 250402 (2012)

### Formalism of sequential measurements

#### Projective measurements

Probabilities are determined by

$$p_i = Tr(\Pi_i \varrho)$$

and the state is transformed via

 $\varrho \mapsto \Pi_i \varrho \Pi_i$ ,

where  $\sum_{i} \Pi_{i} = \mathbb{1}$  and  $\Pi_{i} \Pi_{j} = \delta_{ij} \Pi_{i}$ .

#### POVMs and instruments

Probabilities are determined by

$$p_i = Tr(E_i \varrho)$$

and the state is transformed via

$$\varrho \mapsto \Lambda_i(\varrho),$$

where  $\sum_{i} E_{i} = 1$  and  $E_{i} \ge 0$ .

### Questions for temporal inequalities

- Which resources are needed to classically simulate the quantum violation of such inequalities?
- How can we compute the maximal values for sequential measurements in QM?
- Can we characterize all possible temporal correlations?
- How do the correlations depend on the dimension of the quantum system?

# Classical simulation of Kochen-Specker experiments



# Initial questions

In an experiment, it was found that:

 $\langle \mathcal{X}_{\mathrm{MP}} 
angle = 5.46(4) > 4.$ 



- Is this value surprising?
- Could it be explained by a classical mechanism?
- For instance, if the system remembers the measurements made?
- What memory is required for that?
- Analogous question: What communication is needed to simulate a violation of a Bell inequality?

# Mathematical formulation



• We have an infinite sequence of questions

 $\overleftarrow{\mathcal{Q}} = \{..., Q_{t-1}, Q_t, Q_{t+1}, ...\}$ 

• We obtain an infinite sequence of answers

$$\overleftrightarrow{\mathcal{A}} = \{..., A_{t-1}, A_t, A_{t+1}, ...\}$$

• The questions are chosen randomly from the nine measurements, the answers obey the conditions of the Peres-Mermin square.

### Simulating simple time series

#### Hidden Markov models

- Only one question is allowed  $\Rightarrow$  observe random sequence  $\overleftrightarrow{\mathcal{A}}$
- A HMM has internal states  $i \in \{1, ..., N\}$
- For any state there is an output probability  $A = \{a_{ki}\} = P(A_k|i)$
- In addition, there are transition probabilities  $U = \{u_{ij}\} = P(i \mapsto j|i)$ .
- Finally, one has an initial state distribution  $\pi_i = P(i)$



L. Rabiner, B Juang, IEEE ASSP Magazine, 1986

### Deterministic processes: Mealy machines



#### Ingredients

- A memory that can be in states  $i \in \{1, ..., k\}$
- For any memory state there is a table *A<sub>i</sub>* with the answers to the possible questions.
- For any memory state there is a table  $U_i$ , describing the update rules for the memory, depending on the question.

How many memory states are needed to simulate a given process?

### A simple Mealy machine



 $\begin{aligned} & Q = (a, a, b, b, a, b, a, b, a, a, ...) \\ & S = (1, 1, 1, 2, 2, 3, 1, 1, 2, 3, ...) \\ & A = (+, +, -, -, -, +, +, -, -, -, ...) \end{aligned}$ 

#### $\varepsilon$ -machines

- Consider only one question.
- One can split the answers in past and future

$$\overleftarrow{\mathcal{A}} = \{\dots, A_{-3}, A_{-2}, A_{-1}\}$$
$$\overrightarrow{\mathcal{A}} = \{A_0, A_1, A_2, \dots\}$$

• Two pasts are equivalent, if they predict the same future:

$$\overleftarrow{a} \sim \overleftarrow{a}' \Leftrightarrow P(\overrightarrow{\mathcal{A}} | \overleftarrow{a}) = P(\overrightarrow{\mathcal{A}} | \overleftarrow{a}')$$

- The equivalence classes define the causal states *s*. The output for a given causal state defines transitions between them.
- The statistical complexity is the entropy of the distribution of the  $S = \{s\}$ . This is the memory required for the simulation.

J. P. Crutchfield, Physica D 75, 11 (1994).

#### $\varepsilon$ -transducer

ε

• We consider questions and answers as a single variable:

$$\overleftarrow{\mathcal{Z}} = (\overleftarrow{\mathcal{Q}}, \overleftarrow{\mathcal{A}})$$

• Define equivalence relations for the past outcomes:

$$\overleftarrow{z} \sim \overleftarrow{z}' \Leftrightarrow P(\overrightarrow{\mathcal{A}} | \overrightarrow{\mathcal{Q}}, \overleftarrow{z}) = P(\overrightarrow{\mathcal{A}} | \overrightarrow{\mathcal{Q}}, \overleftarrow{z}')$$

• This defines causal states and the corresponding statistical complexity.

N. Barnett, J. P. Crutchfield, J. Stat. Phys. 161, 404 (2015).

# HMM and arepsilon

#### Properties

- $\varepsilon$ -machines are special HMM.
- $\varepsilon$ -machines are unifilar: The output defines the transition.
- For an ε-machine the state contains no oracular information (information about the future that is not contained in the past)

• In other words: 
$$H(S, \overrightarrow{\mathcal{A}} | \overleftarrow{\mathcal{A}}) = 0.$$

J.P. Crutchfield et al., arXiv:1007.5354

#### Example:Biased flip of a coin

Consider a coin that flips with a certain probability:

$$P(a_1 = T | a_0 = H) = \frac{1}{2} - \epsilon, \qquad P(a_1 = H | a_0 = T) = \frac{1}{2} - \epsilon$$

### Simple example

#### Simulation with an $\varepsilon$ -machine

- The causal states are defined by the last output.
- Both causal states are equally probable.
- 1 bit of complexity/memory.



#### Simulation with HMM

- Three states: fair coin, two completely biased coins.
- If  $\epsilon$  is small: less than one bit.



### Perfect correlations & Mealy machines

#### Correlations to be simulated

- Measurements can be repeated:  $v(A_1|AA) = v(A_2|AA)$  etc.
- The machine reproduces all six Mermin-Peres predictions.
- The observables are compatible in a single sequence:  $v(A_1|ABCA) = v(A_4|ABCA)$  etc.
- The observables fulfil other compatibility constraints, e.g.  $v(A_1|ACaA) = v(A_4|ACaA)$ .

• ...

• The machine reproduces all quantum predictions.

$$\begin{bmatrix} A & B & C \\ a & b & c \\ \alpha & \beta & \gamma \end{bmatrix}$$

### Four-state Mealy machine

• Consider the following four  $A_i$  and the update tables  $U_i$ :

 $\begin{bmatrix} - & - & + \\ - & - & + \\ + & + & + \end{bmatrix} \begin{bmatrix} + & - & + \\ + & - & - \\ + & + & + \end{bmatrix} \begin{bmatrix} - & + & + \\ - & - & + \\ + & - & - \end{bmatrix} \begin{bmatrix} + & + & + \\ + & - & - \\ + & - & - \end{bmatrix}$  $U_1: \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 3 \\ 0 & 0 & 2 \end{bmatrix} U_2: \begin{bmatrix} 4 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} U_3: \begin{bmatrix} 1 & 4 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} U_4: \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 0 & 3 \end{bmatrix}$ 

- This machine predicts:  $C_{(1)}^+ c_{(1)}^+ \gamma_{(3)}^- C_{(3)}^+ B_{(3)}^+ A_{(4)}^+ c_{(4)}^- A_{(2)}^+ \dots$
- It reproduces all deterministic predictions of QM for the PM square.
- Machines with three states cannot do this, so it is optimal.
- Can all two-qubit effects be simulated with two bits of memory?

M. Kleinmann et al., New J. Phys. 13, 113011 (2011), see also P. Blasiak, Ann. Phys. 353, 326 (2015) G. Fagundes, et al., arXiv:1611.07515.

### Improving the Peres-Mermin square

#### Question

Are there KS inequalities for qubits with a higher violation?



Using all Pauli matrices one can find a correlation with  $\langle \chi_{MP} \rangle =$  15 (in QM), but for noncontextual theories:  $\langle \chi_{MP} \rangle \leq$  9.

A. Cabello, Phys. Rev. A 82, 032110 (2010)

#### Theorem

Simulating this extended PM square for two qubits requires more than two classical bits as a memory.

#### Consequence

Two qubits can store only to classical bits, but for simulating deterministic two-qubit effects more than two bits of memory are needed.

M. Kleinmann et al., New J. Phys. 13, 113011 (2011)

### Simulating quantum predictions: $\varepsilon$ -transducer



- Measuring a sequence or row projects the system in one of 24 quantum states.
- These are the causal states of the  $\varepsilon$ -transducer.

A. Cabello, M. Gu, O Gühne, in preparation

### Simulating quantum predictions: $\varepsilon$ -transducer



- From the Yu-Oh measurements, one obtains an infinite set of quantum states.
- Does an  $\varepsilon$ -transducer require an infinite amount of memory?

# Bounding temporal correlations



### Bounding temporal quantum correlations



#### Question

What are the maximal quantum values for temporal correlations?

#### Crucial assumption

In this part, we only consider projective measurements, e.g.,

$$A_i = \Pi_i^+ - \Pi_i^-$$

However, it is not assumed that measurements are dichotomic or commute.

# Simple method

• For dichotomic observables, one has

$$\langle A_i A_j \rangle_{seq} = \frac{1}{2} [Tr(\varrho A_i A_j) + Tr(\varrho A_j A_i)]$$

• Define a matrix

$$X_{ij} = \langle A_i A_j \rangle_{\mathrm{seq}}$$

This is real, symmetric, positive and  $X_{ii} = 1$ 

- Maximizing the quantum value is equivalent to maximizing  $C = \sum_{ij} \lambda_{ij} X_{ij}$ .
- This can be solved with an semidefinite program, often also analytically.

S. Wehner, PRA 2006; T. Fritz, NJP 2010, C. Budroni et al., PRL 2013

### Application to the Leggett-Garg inequality



# Second method

- Denote settings by  $\mathbf{s} = (s_1, s_2, \dots, s_n)$  and results by  $\mathbf{r} = (r_1, r_2, \dots, r_n)$ .
- The sequential mean value is a function of the probabilities

 $P(\mathbf{r}|\mathbf{s}) \equiv P_{\text{seq}}(r_1, r_2, \ldots, r_n|s_1, s_2, \ldots, s_n).$ 

which can be computed with the projector  $\Pi(\mathbf{r}|\mathbf{s}) = \prod_{r_1}^{s_1} \prod_{r_2}^{s_2} \dots \prod_{r_n}^{s_n}$ .

• Consider the matrix of moments

$$M_{\mathbf{r}|\mathbf{s};\mathbf{r}'|\mathbf{s}'} = \langle \Pi(\mathbf{r}|\mathbf{s})\Pi(\mathbf{r}'|\mathbf{s}')^{\dagger}|. \rangle$$

• Again, the maximum can be computed with a semidefinite program (the first step of the NPA hierarchy)

C. Budroni et al., Phys. Rev. Lett. 111, 020403 (2013)

### Application to Yu & Oh & other inequalities



Ineq.	NCHV	State-independent	Algebraic	Sequential
	bound	quantum value	maximum	bound
Yu-Oh	16	50/3pprox 16.67	50	17.794
Opt2	16	52/3 pprox 17.33	52	20.287
Opt3	25	$83/3 \approx 27.67$	65	32.791

S. Yu et al., PRL 2012, M. Kleinmann et al., PRL 2012

# General temporal correlations



### General temporal correlations

#### Question

Can we characterize all the probabilities coming from sequential quantum measurements?

#### Properties

• Consider sequences of length k and the set of all probabilities

$$p(x, y, z, \ldots | X, Y, Z, \ldots).$$

• The probabilities have to obey the arrow of time (AoT):

$$p(a,\cdot|AB) = p(a,\cdot|AA)$$

• How does this set look? What are the quantum mechanically allowed probabilities?

L. Clemente, J. Kofler, Phys. Rev. Lett. 116, 150401 (2016)

### General temporal correlations



Picture from L. Clemente, J. Kofler, Phys. Rev. Lett. 116, 150401 (2016)





#### Result 1

The extremal points of the temporal correlation polytope are exactly the deterministic assignments that obey AoT.

#### Result 2

All extremal points can origin from QM, but they may require general measurements and high-dimensional systems

#### Result 3

Some simple extremal points cannot origin from two-dimensional systems.

J. Hoffman, MSc thesis, T. Fritz, NJP 2010, L. Clemente et al., PRL 2016



• Consider two measurements with two outcomes and then:

T = p(+ - |AA) + p(+ + |AB) + p(- + |BA) + p(- + |BB)

- We can reach T = 4 with a deterministic AoT assignment.
- For qubits: If p(+ |AA) = p(- + |BB) = 1 the measurements must be projective. But then p(+ + |AB) = p(- + |BA) = 1 cannot be reached.

• We have the inequality

$$T \stackrel{2D}{\leq} 3.18623 \stackrel{3D}{\leq} 4$$

• This may be tested experimentally ...

J. Hoffmann et al., in preparation.



#### Results

- Sequential measurements are essential for tests of quantum contextuality.
- The classical resources for simulating the PM square can be quantified.
- One can compute temporal Tsirelson bounds with SDP.
- Temporal quantum correlations can be used for certifying the dimension of quantum systems



