

Closing the Problem of Classical-Quantum Gaps in Causal Structures:

Which causal structures of up to six nodes support non-classical quantum correlations?

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Outline

- 1 Introduction: Understanding Causality
- 2 Main Result: The Causal Structure G_1
- 3 Generalization: Other Causal Structures
- 4 Completing the Classification
- 5 Conclusions

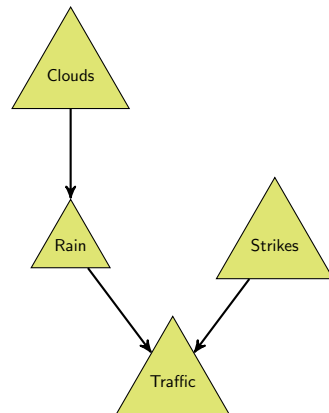
Motivation: Why Study Causality?

Everyday causality:

- Clouds cause rain
- Rain causes traffic delays
- Strikes cause traffic delays

Key question:

Can we represent these relationships formally?



Goal

Develop a mathematical framework to represent and analyze causal relationships.

Causal Structures: Directed Acyclic Graphs (DAGs)

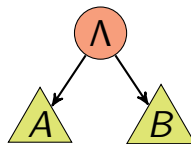
Definition

A **causal structure** (or DAG) is a directed acyclic graph where:

- **Nodes** represent variables (events, measurements)
- **Directed edges** represent *possible* direct causal influences
- **No cycles** (acyclic): cannot return back to the same node following a (directed) path formed by directed edges.

Two types of nodes:

- **Observed** (triangles): We can measure these variables
- **Latent** (circles): Hidden, unobserved variables



The Causal Markov Condition

How do causal structures constrain probability distributions?

Causal Markov Condition

A probability distribution $P(X_1, \dots, X_n)$ is **classically compatible** with a DAG iff it factorizes as:

$$P(x_1, \dots, x_n) = \prod_{i=1}^n P(x_i \mid \text{parents}(X_i)).$$

Interpretation: Each variable is independent of its indirect causes and non-causes (non-descendants) given its direct causes (parents).

Simple Example

For Clouds \rightarrow Rain \rightarrow Traffic:

$$P(\text{clouds}, \text{rain}, \text{traffic}) = P(\text{clouds}) \cdot P(\text{rain} \mid \text{clouds}) \cdot P(\text{traffic} \mid \text{rain}).$$

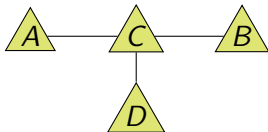
d-separation: Reading Off Independencies

The DAG structure tells us which variables are independent!

d-separation

A graphical criterion to determine conditional independencies from the DAG structure alone.

Example:



Independencies:

- $A \perp B \mid C$
(Given C , A and B are independent)
- $A \perp D \mid C$
- But $A \not\perp B$ unconditionally

Key insight: The graph structure determines which correlations are possible.

Classical vs. Quantum: What's the Difference?

Different theories allow different types of correlations!

Classical Theory:

- Latent nodes = random variables
- Observed nodes = random variables
- Joint distribution satisfies Causal Markov condition
- Set of allowed distributions: \mathcal{C}

Quantum Theory:

- Latent nodes = quantum states
- Observed nodes = quantum measurements (POVMs)
- Joint distribution obtainable from the Born Rule
- Set of allowed distributions: \mathcal{Q}

The hierarchy of the possible sets of distributions

$$\mathcal{C} \subseteq \mathcal{Q} \subseteq \mathcal{G} \subseteq \mathcal{I}$$

where \mathcal{G} = set of correlations obtainable in any Generalised Probabilistic Theory, \mathcal{I} = set of correlations satisfying only the observed conditional independences (weakest constraints).

Classical vs. Quantum in arbitrary causal structures

Central Question

For which causal structures is $\mathcal{C} \subsetneq \mathcal{Q}$? (Classical-quantum gap?)

An easier question

For which causal structures is $\mathcal{C} \subset \mathcal{I}$?

Because if $\mathcal{C} = \mathcal{I}$ then trivially $\mathcal{C} = \mathcal{Q}$.

Bell's Theorem: The First Classical-Quantum Gap (C-Q gap)

Bell (1964): Quantum mechanics violates Local Causality (under the assumption of measurement independence)

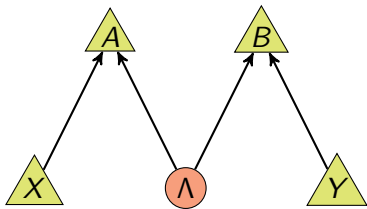


Figure: The Bell DAG

Classical factorization:

$$P(a, b, x, y) = \sum_{\lambda} Q(a|x, \lambda) Q(b|y, \lambda) Q(x) Q(y) Q(\lambda).$$

This is **local causality**.

Bell's Result

Classical distributions (where sources are hidden variables) satisfying this must obey Bell inequalities. But quantum mechanics can violate them! Hence $\mathcal{C} \subsetneq \mathcal{Q}$ for the Bell DAG.

What are Classical and Quantum distributions in the Bell Causal Structure: An example for sets \mathcal{C} and \mathcal{Q}

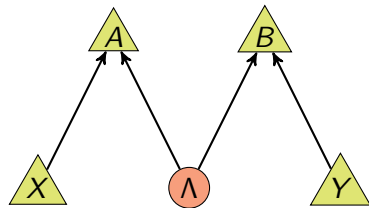


Figure: The Bell DAG

By Bell's theorem $\mathcal{C} \subset \mathcal{Q}$ and therefore there is a Classical-Quantum gap in the Bell DAG.

The set of Classically compatible distributions is:

$$\mathcal{C} = \left\{ P(a, b, x, y) : P(a, b, x, y) = \sum_{\lambda} Q(a | x, \lambda) Q(b | y, \lambda) Q(x) Q(y) Q(\lambda) \right\}$$

The set of Quantum Mechanically compatible distributions is:

$$\mathcal{C} = \left\{ P(a, b, x, y) : P(a, b, x, y) = \text{Tr}(\rho_{AB} E_x^A \otimes E_y^B) P(x)P(y) \right\}$$

Beyond Bell: Which Other Structures Have a C-Q Gap?

Are there other causal structures with classical-quantum gaps?

- **Fritz (2012):** Triangle scenario has a gap
- **HLP (2014):** Classified 366,565 causal structures with ≤ 6 nodes
 - Showed 366,565 – 21 (*modulo redundancies*) structures have **no C-Q gap**
 - Left 21 candidates that *could* have a C-Q gap

Prior to this work

Known gaps: Bell, Instrumental, Triangle, Unrelated Confounders (*special names given to certain causal structures*)

Progress: Following the technique of Fritz, 16 more shown by Fox et al. (upcoming)

Remaining: Only 1 open case for ≤ 6 nodes (our focus!)

Our Contribution

We resolve the last open case, completing the classification for all causal structures with ≤ 6 nodes!

The Remaining Open Case: G1

Causal structure G1:

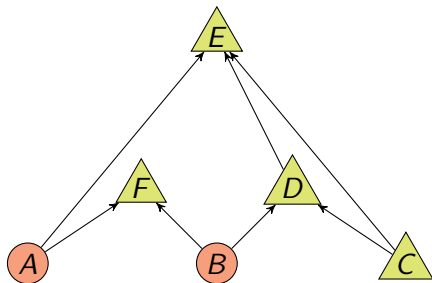


Figure: The causal structure G_1 that is the focus of this work.

Challenge:

- 2 latent nodes: A, B
- 4 observed nodes: C, D, E, F
- Complex connectivity
- Standard techniques don't work

Question:

Does G_1 support quantum correlations that cannot be realized classically?

Our Main Theorem

Yes! There exist quantum correlations compatible with G_1 that have no classical explanation within G_1 .

Our Strategy: Imposing Additional Conditions

Key insight: Consider a restricted subset of correlations

Additional Conditions

- 1 **Variable splitting:** Let $F = (F_O, F_S)$ where $F_S = E$ always
- 2 **Independence:** Let E be independent of C and D in the observed distribution, i.e., $P(e|cd) = P(e)$

What do these conditions achieve?

- Force E to be determined entirely by A (not influenced by C or D)
- Effectively “turn off” the causal links $C \rightarrow E$ and $D \rightarrow E$
- Make E independent of B (**the most important part**)
- Create a Bell-like structure hidden within G1!

Strategy

- 1 Show: Classical + Conditions 1,2 \Rightarrow Bell's local causality
- 2 Construct: Quantum correlations violating this (using entanglement)

Classical Compatibility with G1

What does it mean for correlations to be classically compatible with G1?

Definition: Classical Compatibility

$P(CDEF)$ is classically compatible with G1 if \exists a joint distribution $Q(ABCDEF)$ such that:

$$P(cdef) = \sum_{a,b} Q(abcdef)$$

$$\text{where } Q(abcdef) = Q(a)Q(b)Q(c)Q(d|bc)Q(e|acd)Q(f|ab)$$

Interpretation:

- Each term $Q(x_i|\text{parents}(X_i))$ reflects direct causal influence
- Marginalization over latent variables A, B gives observed distribution

Quantum Compatibility with G1

In the quantum case, latent nodes are quantum states

Definition: Quantum Compatibility

$P(CDEF)$ is quantum mechanically compatible with G1 if there exist:

- Hilbert spaces $H_A^E, H_A^F, H_B^F, H_B^D$
- Quantum states ρ_A on $H_A^E \otimes H_A^F$ and ρ_B on $H_B^F \otimes H_B^D$
- POVMs (measurements):
 - $\{K_d^c\}_d$ on H_B^D (for each c)
 - $\{M_e^{c,d}\}_e$ on H_A^E (for each c, d)
 - $\{N_f\}_f$ on $H_A^F \otimes H_B^F$

such that:

$$P(cdef) = \text{tr} \left((M_e^{c,d} \otimes N_f \otimes K_d^c) (\rho_A \otimes \rho_B) \right) P(c)$$

Key: Node B can hold an entangled state!

Lemma 1: Classical Case Reduces to Bell Scenario

With our additional conditions, classical correlations must satisfy Bell's local causality form

Lemma 1 (Classical + Conditions \Rightarrow Local Causality)

If $P(CDEF)$ is classically compatible with G1 and satisfies Conditions 1 and 2, then:

$$P(cdef_O) = \sum_b Q(b)Q(c)Q(e)Q(d|bc)Q(f_O|be).$$

Key observations:

- This is exactly Bell's local causality form!
- "Settings": E (determined by A) and C
- "Outcomes": F_O and D
- Shared common cause: B

Proof approach:

- 1 Start with classical factorization from G1
- 2 Apply d-separation relations:
 $F \perp CD|B, E \perp B|CD, B \perp C$
- 3 Use Conditions 1 and 2 to simplify

Proof Sketch of Lemma 1 (Part 1)

Step 1: Start with classical compatibility

$$\begin{aligned} P(cdef) &= \sum_{a,b} Q(abcdef) \\ &= \sum_{a,b} Q(b)Q(c|b)Q(d|bc)Q(e|bcd)Q(f|bcde)Q(a|bcdef) \end{aligned}$$

Step 2: Apply d-separation relations from Theorem 1:

- $F \perp CD|B \Rightarrow Q(f|bcd) = Q(f|b)$
- $E \perp B|CD \Rightarrow Q(e|bcd) = Q(e|cd)$
- $B \perp C \Rightarrow Q(c|b) = Q(c)$

This gives:

$$P(cdef) = \sum_b Q(b)Q(c)Q(d|bc)Q(e|cd)Q(f|bcde)$$

Proof Sketch of Lemma 1 (Part 2)

Step 3: Apply Condition 2: $P(e|cd) = P(e)$

Since $P(e|cd) = \sum_b Q(b)Q(d|bc)Q(e|cd)/(\sum_b Q(b)Q(d|bc))$, we get $Q(e|cd) = Q(e)$

Step 4: Apply Condition 1: $F = (F_O, F_S)$ with $F_S = E$

Replace f with $f_O f_S$ and sum over f_S :

$$P(cdef_O) = \sum_{b, f_S} Q(b)Q(c)Q(d|bc)Q(e)Q(f_O f_S|bcde)$$

Step 5: Simplify using $F_S = E$, $F = (F_S, F_O) = (E, F_O)$

Since $Q(ef_O|bcd) = Q(f_O f_S|bcd) = Q(f|bcd) = Q(f|b) = Q(e|b)Q(f_O|be) = Q(e)Q(f_O|be)$,
(using $Q(e|bcd) = Q(e)$ and $Q(e|cd) = Q(e) \implies Q(e|b) = Q(e)$) we get:

$$P(cdef_O) = \sum_b Q(b)Q(c)Q(e)Q(d|bc)Q(f_O|be)$$

This is Bell's local causality form!

The CHSH Inequality

Bell's local causality implies testable constraints

CHSH Inequality (Clauser, Horne, Shimony, Holt 1969)

For any distribution of the form $P(ab|xy) = \sum_{\lambda} Q(a|x, \lambda)Q(b|y, \lambda)Q(\lambda)$:

$$P(A = B|00) + P(A = B|01) + P(A = B|10) + P(A \neq B|11) \leq 3$$

In our case:

- Settings: E and C (binary)
- Outcomes: F_O and D (binary)
- If classical + Conditions 1,2 hold, then:

$$P(D = F_O|00) + P(D = F_O|01) + P(D = F_O|10) + P(D \neq F_O|11) \leq 3$$

Strategy: Construct quantum correlations that violate this!

Lemma 2: Quantum Violation

Construction using entanglement:

Define $|\theta\rangle = \cos(\theta)|0\rangle + \sin(\theta)|1\rangle$

- ① A : uniformly random classical bit or $A = \frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|11\rangle\langle 11|$
- ② $\rho_B = |\Psi^+\rangle\langle\Psi^+|$ where $|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ (maximally entangled!)
- ③ C : uniformly random classical bit, i.e., $P(C = 0) = P(C = 1) = 0.5$
- ④ $F_S = A$, and F_O is outcome of measuring H_B^F in basis:
 - $\{|0\rangle, |\pi/2\rangle\}$ if $F_S = 0$
 - $\{|\pi/4\rangle, |3\pi/4\rangle\}$ if $F_S = 1$
- ⑤ D is outcome of measuring H_B^D in basis:
 - $\{|\pi/8\rangle, |5\pi/8\rangle\}$ if $C = 0$
 - $\{|-\pi/8\rangle, |3\pi/8\rangle\}$ if $C = 1$
- ⑥ $E = A = F_S$ by both E and F_S measuring $H_A^E, H_A^{F_S}$ in the computational basis $\{|0\rangle, |1\rangle\}$

Result: Standard CHSH calculation gives:

$$P(D = F_O|00) + P(D = F_O|01) + P(D = F_O|10) + P(D \neq F_O|11) = 4 \cos^2(\pi/8) \approx 3.41$$

Obtained distribution violates CHSH! \Rightarrow Classically infeasible in G1

The Probability Distribution

c	e	f_O	d	$P(cefd)$
0	0	0	0	$\cos^2(\pi/8) \approx 0.116$
0	0	0	1	$\sin^2(\pi/8) \approx 0.009$
0	0	1	0	$\sin^2(\pi/8) \approx 0.009$
0	0	1	1	$\cos^2(\pi/8) \approx 0.116$
0	1	0	0	$\cos^2(\pi/8) \approx 0.116$
0	1	0	1	$\sin^2(\pi/8) \approx 0.009$
0	1	1	0	$\sin^2(\pi/8) \approx 0.009$
0	1	1	1	$\cos^2(\pi/8) \approx 0.116$
1	0	0	0	$\cos^2(\pi/8) \approx 0.116$
1	0	0	1	$\sin^2(\pi/8) \approx 0.009$
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1	1	1	0	$\cos^2(\pi/8) \approx 0.116$
1	1	1	1	$\sin^2(\pi/8) \approx 0.009$

Table: Quantum correlations for G1 violating the corresponding CHSH inequality (omitting f_S since $f_S = e$).

Summary of Main Result

Theorem (Main Result)

There exist quantum correlations compatible with G1 that cannot be realized classically in G1.

Proof strategy:

- ① Impose additional conditions that:
 - Isolate a Bell-like substructure
 - Don't necessarily use all causal links
- ② Show classical + conditions \Rightarrow Bell local causality (Lemma 1)
- ③ Construct quantum correlations using entanglement that violate CHSH (Lemma 2)
- ④ Conclude: These quantum correlations have no classical explanation in G1

Application of our strategy

Our method of imposing additional conditions to reveal hidden Bell structures works beyond G1!

Causal structure G2:

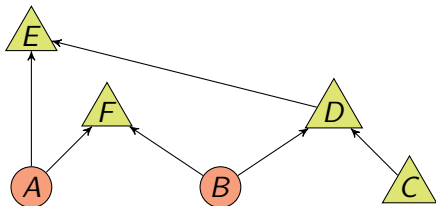


Figure: $G1 = G2$ without $C \rightarrow E$

Immediate corollary:

- Our quantum construction for G1 didn't use the link $C \rightarrow E$
- These same correlations work for G2
- Removing an edge adds constraints
- Hence, the classical set for $G2 \subset$ classical set for G1

Result

G2 also has a classical-quantum gap!

The Triangle Causal Structure

Triangle structure:

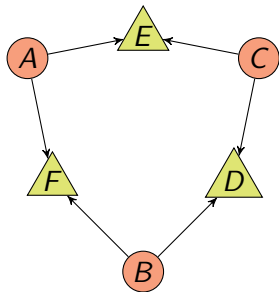


Figure: The triangle causal structure.

Fritz's result (2012):

- Showed that the triangle causal structure has a classical-quantum gap
- Used entropy-based arguments to show this

Our contribution:

- Alternative proof at the level of probabilities using our technique
- More direct construction and easier to follow

Method: Take $D = (S_1, O_1)$, $E = (S'_1, S'_2)$, $F = (S_2, O_2)$ with $S'_1 = S_1$ and $S'_2 = S_2$. Then classical compatibility reduces to Bell local causality!

Generalizing the “Fritz Trick”

Our method extends Fritz’s approach:

The General Strategy

- ① Identify potential “settings” and “outcomes” in the causal structure
- ② Impose conditions that:
 - Turn off interfering causal paths. If need be consider perfectly correlated bits.
 - Create independence structure mimicking Bell scenario
 - Force settings to be independent of the latent common cause of the outputs
- ③ Prove: Classical + conditions \Rightarrow local causality form
- ④ Construct: Quantum violations using entanglement

Key insight: Work at the level of probabilities, not entropies

- More direct and easier to follow
- Easier to construct explicit quantum violations
- Generalizes more naturally

The Big Picture: All Structures up to 6 Nodes

The journey to complete classification:

- **Total:** 366,565 causal structures with ≤ 6 nodes
- **HLP (2014):** Ruled out 366,544 (no gap possible or any possible gap can be reduced to the remaining 21)
- **Remaining:** 21 candidates

Resolution of the 21 Cases

Bell (1964):	Bell DAG
Fritz (2012):	Triangle
Instrumental (2018-19):	Instrumental scenario
Unrelated Confounders (2024):	Simplest causal network
Fox et al. (upcoming):	Following the technique of Fritz, 16 more cases out of the 21 remaining
This work (2025):	G1 (the last case!)

Post-Quantum Correlations

Can we go beyond quantum mechanics?

Hierarchy of Correlation Sets

$$\mathcal{C} \subseteq \mathcal{Q} \subseteq \mathcal{G} \subseteq \mathcal{I}$$

- \mathcal{C} : Classical (local hidden variables)
- \mathcal{Q} : Quantum (entanglement, measurements)
- \mathcal{G} : Generalised Probabilistic Theories
- \mathcal{I} : Graph-compatible (respects DAG observed conditional independencies)

Question: Are there structures where $\mathcal{Q} \subsetneq \mathcal{G}$ (post-quantum correlations) such that $\mathcal{C} \subseteq \mathcal{Q}$?

Result from our work

For ≤ 6 nodes: No! Every structure with potential of $\mathcal{Q} \subsetneq \mathcal{G}$ also necessarily has $\mathcal{C} \subsetneq \mathcal{Q}$.
There are no structures with post-quantum but not non-classical quantum correlations.

Why does this matter?

Foundational:

- Deeper understanding of causality at the level of quantum mechanical systems
- Shows quantum non-classicality is not limited to the Bell causal structure
- No post-quantum correlations without non-classical quantum correlations (for ≤ 6 nodes), indicating the same might be true for larger DAGs

Practical:

- Identifying which experiments can demonstrate quantum advantage
- Causal inference with quantum resources
- Quantum cryptography beyond standard settings

Summary

- ① **Resolved the last open case:** Showed G1 has a classical-quantum gap
- ② **New methodology:** Developed a technique of imposing additional conditions to reveal hidden Bell structure in other structures
- ③ **Complete classification:** All causal structures with ≤ 6 nodes now classified
- ④ **Generalized Fritz's approach:** Applied to multiple structures (G1, G2, Triangle)
- ⑤ **No post-quantum without quantum:** Ruled out intermediate theories for ≤ 6 nodes

Future Directions and Applications

- Experimental demonstrations of quantum violations in different structures
- Causal discovery with quantum data
- Quantum network protocols
- Device-independent applications
- Develop systematic algorithms for finding quantum violations
- Explore connections to other areas such as machine learning and causal inference)

For details, please refer:

1) Chapter 6 in Khanna, S. (2025). *Exploring non-classical correlations in causal scenarios* (Doctoral dissertation, University of York).

https://etheses.whiterose.ac.uk/id/eprint/36307/1/PhD_Thesis_Submitted_Version.pdf

2) Khanna, S., Pusey, M., Colbeck, R. (2025). *Closing the problem of which causal structures of up to six total nodes have a classical-quantum gap.*

arXiv preprint [arXiv:2512.04058](https://arxiv.org/abs/2512.04058)

<https://arxiv.org/pdf/2512.04058>

Thank You!

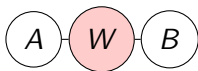
Questions?

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Backup: d-separation in Detail

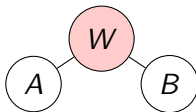
Three types of paths that can be blocked:

Chain:



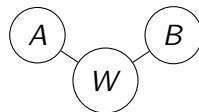
$$A \perp B | W$$

Fork:



$$A \perp B | W$$

Collider:



$A \perp B$ (unconditionally!)
But conditioning on W or
any of its descendants
opens the path

Backup: Full Classical Factorization for G1

Detailed expansion:

Starting from:

$$Q(abcdef) = Q(a)Q(b)Q(c)Q(d|bc)Q(e|acd)Q(f|ab)$$

Expand using conditional probability:

$$\begin{aligned} P(cdef) &= \sum_{a,b} Q(abcdef) \\ &= \sum_{a,b} Q(b)Q(c|b)Q(d|bc)Q(e|bcd)Q(f|bcde)Q(a|bcdef) \end{aligned}$$

Apply d-separations:

- $B \perp C \Rightarrow Q(c|b) = Q(c)$
- $E \perp B|CD \Rightarrow Q(e|bcd) = Q(e|cd)$
- $F \perp CD|B \Rightarrow Q(f|bcd) = Q(f|b)$

Result:

$$P(cdef) = \sum Q(b)Q(c)Q(d|bc)Q(e|cd)Q(f|bcde)$$