Contextuality and quantum simulation of Pauli Hamiltonians

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IBM Quantum

(work conducted at Tufts University with Peter Love

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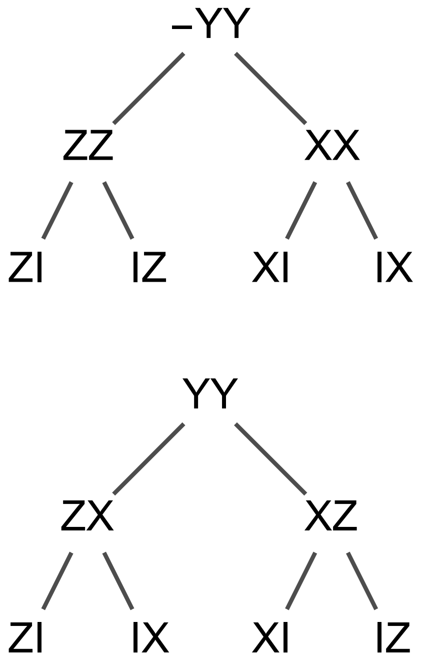

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Motivation

Studying measurements of collections of Pauli operators.

- Most typical basis for measuring observables in near term
- Even many LCU/block encoding constructions start with Pauli decomposition

Typical task: repeatedly run same circuit and measure different Pauli operators in observable

$$H = \sum_i \alpha_i P_i$$

Pauli operators review

- Notation: $\sigma_x \otimes \sigma_z = XZ$
- Self-inverse (eigenvalues ± 1)
- Basis for Hermitian operators
- Local Hamiltonians = linear combinations of $poly(n)$ Pauli operators
- Either commute or anticommute:

e.g. XX, ZZ commute, XX, ZX anticommute

- Products are Pauli operators up to phase:

e.g. $(XX)(ZZ) = -YY$

Motivating question

When can we describe a set of Pauli observables “classically”?

- Need to pick a notion of classicality.
- Want notion of classicality to hold for any state (e.g., rules out stabilizer subtheory).
- Want notion to hold for any actions of observer/experimenter:
    - Restriction is on what set our model describes…
    - Observer could measure other Pauli operators not in our chosen set.
- Specific meaning of classicality we will use is noncontextual hidden-variable model.

Noncontextual hidden-variable model

Two components:

1. Collection of joint value assignments to observables in set.
2. Collection of probability distributions over joint value assignments.

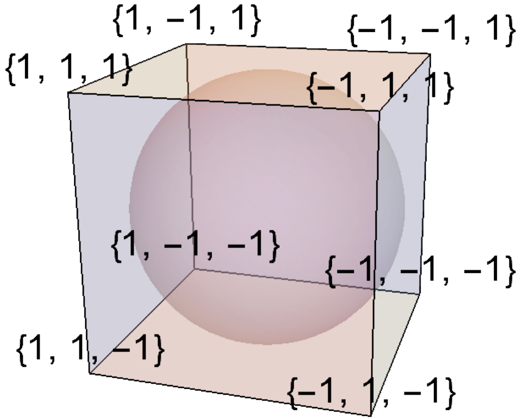
Given such a model, can interpret observables as having real, classical values at all times, which are revealed by measurements, with probability distributions describing our knowledge (or lack thereof).

Noncontextual hidden-variable model

Example:

Single qubit Paulis X, Y, Z

- Joint value assignments ~ corners of cube
- Joint probability distributions:
    - Corner ~ probability 1 for corresponding value assignment
    - Other points correspond to convex combinations of corners
    - Physically allowed probability distributions correspond to points in sphere



Contextual sets

Set of Pauli operators is *contextual* if impossible to build a noncontextual HVM for it.

Recall…

- We wanted two features for our notion of classicality: state independence and “observer freedom”
- The latter will be important for our specific type of contextuality.

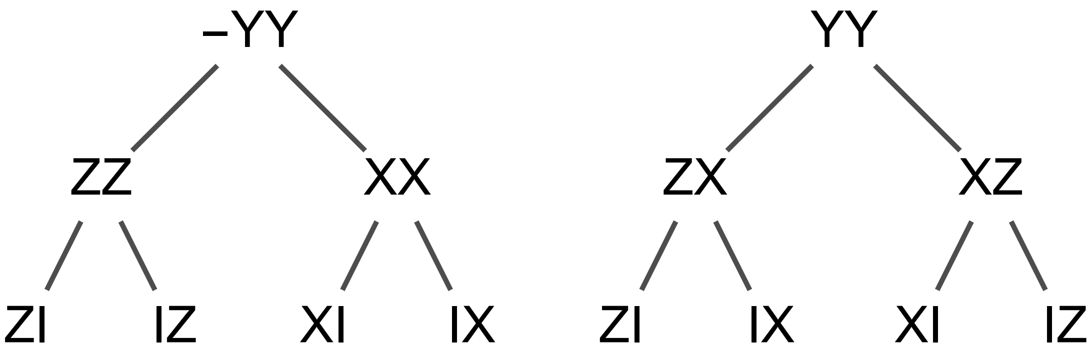
So, what could be an obstacle to constructing noncontextual HVM satisfying the above?

Example (Peres-Mermin square)

Suppose set is XI, IX, ZI, IZ

Observer is free to perform any physically-possible measurements.

⇒ Given a value assignment, can infer values assigned to additional observables below:



−YY

ZZ XX

ZI IZ XI IX

YY

ZX XZ

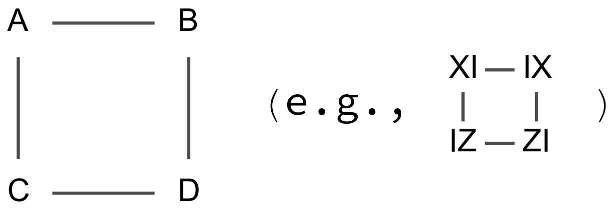
ZI IX XI IZ

Value assignments must be noncontextual, i.e., cannot depend on observer’s choice of measurement.

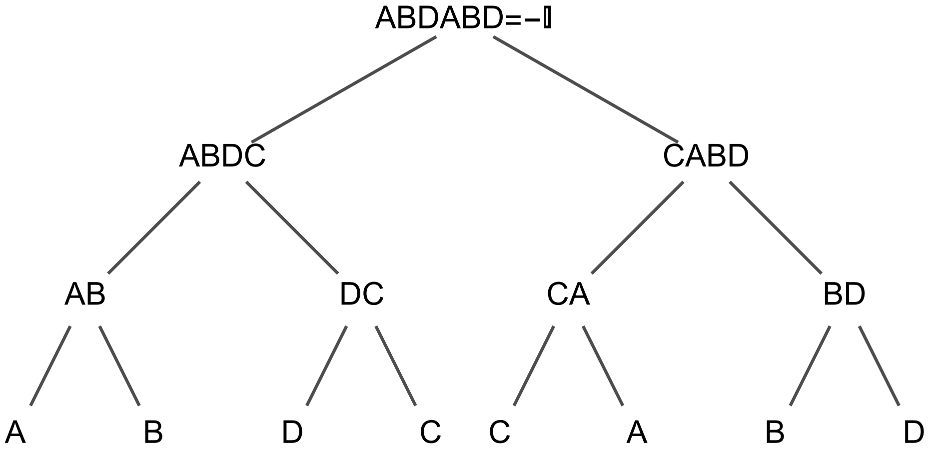
⇒ All value assignments in model must satisfy above inference relations. But this is impossible!

Generalization

For any Paulis A, B, C, D with commutation graph

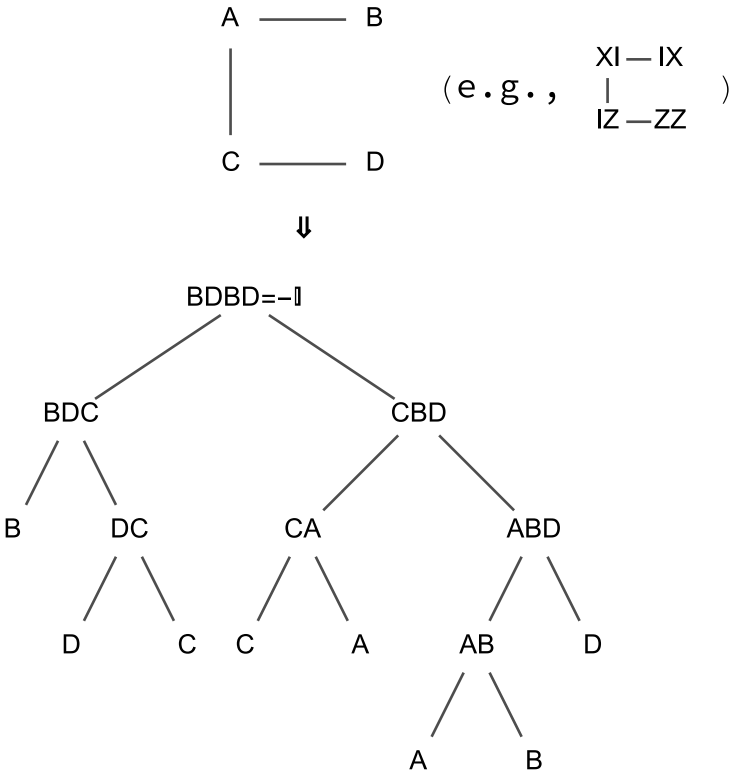


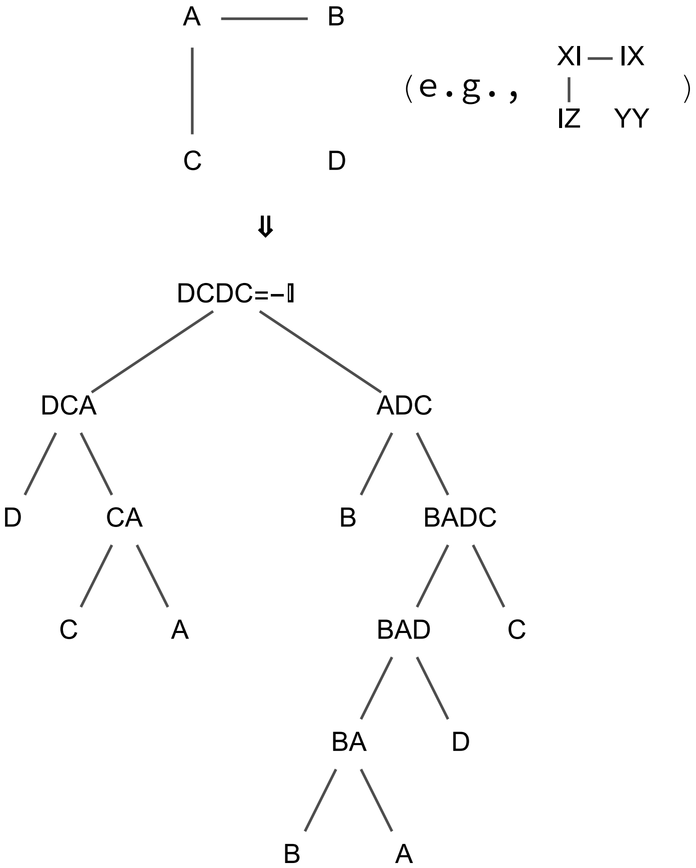
$\Downarrow$



Further generalization

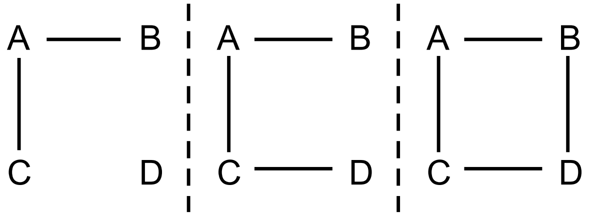
Same holds for two other commutation graphs:





And that's basically it

Theorem [KL19]. A set of Pauli operators is *contextual* if and only if it contains a subset A, B, C, D with one of the following commutation graphs:



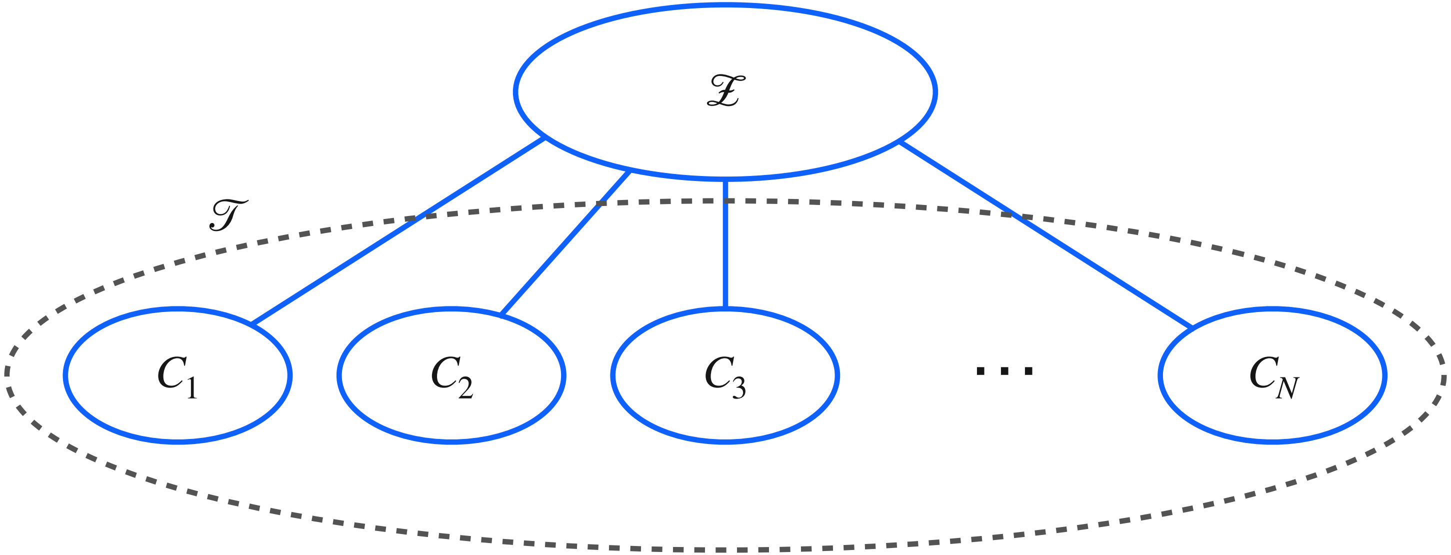
Equivalently, a set $\mathscr{S}$ of Pauli operators is *noncontextual* if and only if it has the form

$$\mathscr{S} = \mathscr{Z} \cup \mathscr{T}$$

where…

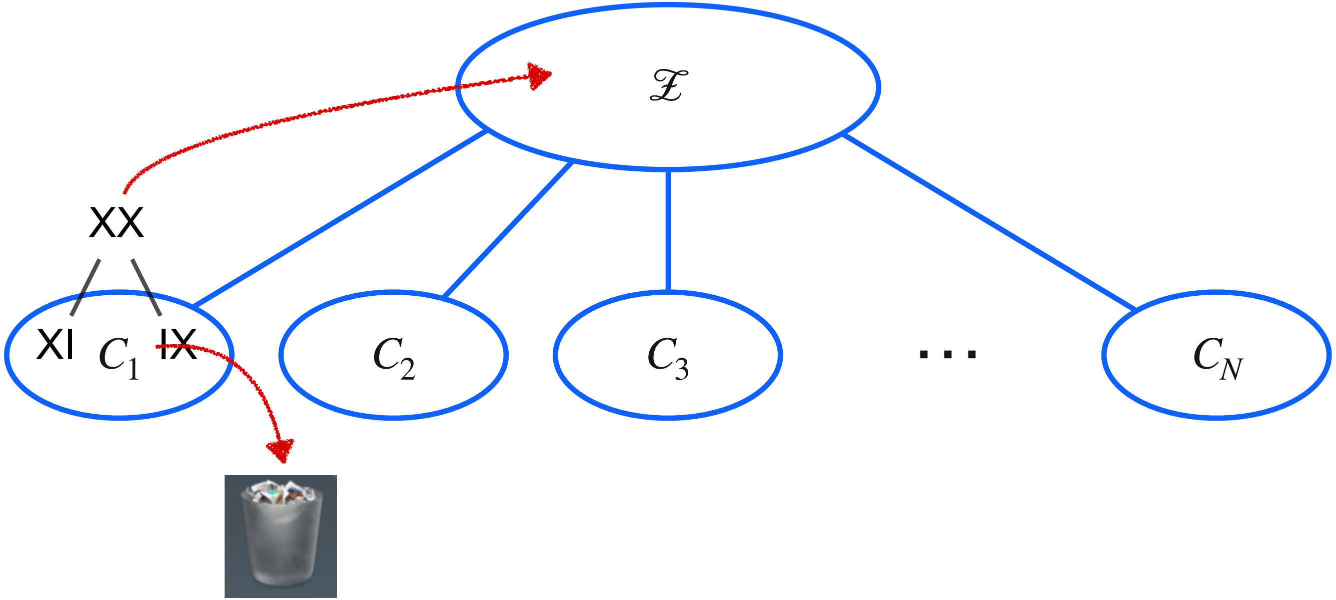
- $\mathscr{Z}$ is the "center" of $\mathscr{S}$, i.e., contains all operators in $\mathscr{S}$ that commute with all others.
- Commutation is an equivalence relation (transitive) on $\mathscr{T}$

A generic noncontextual set of Pauli operators



- Operators in $\mathscr{Z}$ commute with everything.
- Operators in the same C_i commute.
- Operators in different C_i anticommute.

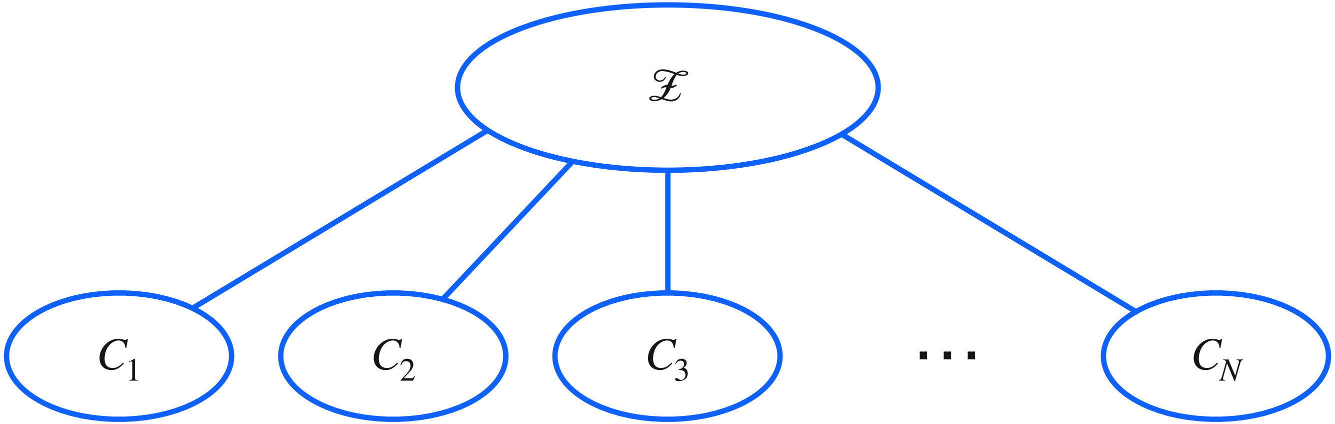
A standard generating set



Repeat: end up with one element in each C_i plus expanded $\mathcal{Z}$

— all Paulis in original set generated by inference.

A standard generating set



Now each C_i is a single Pauli, $\mathscr{Z}$ is a set of commuting Paulis

⇒ can find an independent generating set for $\overline{\mathscr{Z}}$: call its elements G_j

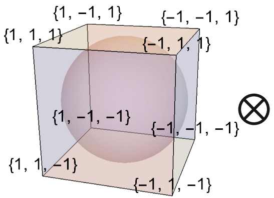
⇒ generic noncontextual Hamiltonian:

$$H = \sum_{B\in\mathscr{Z}} \alpha_B \prod_{j\in\mathscr{J}_B} G_j + \sum_{B\in\mathscr{Z}} \prod_{j\in\mathscr{J}_B} G_j \sum_{i=1}^{N} \alpha_{B,i} C_i \quad = \quad \sum_{B\in\mathscr{Z}} \left(\alpha_B + \sum_{i=1}^{N} \alpha_{B,i} C_i \right) \prod_{j\in\mathscr{J}_B} G_j$$

A standard generating set

Any anticommuting set satisfies $\sum_i \langle P_i \rangle^2 \leq 1$, with equality when the set is maximal and the state is pure.

- I.e., anticommuting sets of Pauli operators look like Bloch spheres, just potentially in more than 3 dimensions.



⇒ generic noncontextual generating set: ⊗ commuting set

Two types of sets that we already knew were classical.

⇒ Under our assumption of "observer freedom" (i.e., inference outside the original set is possible), you can't get anything else and remain noncontextual.

3-qubit example: $\underbrace{XII, YII, ZII}_{\text{anticommute}}, \underbrace{IZI, IIZ}_{\text{commute}}$

What are computational implications?

For a noncontextual set, can construct noncontextual HVM!

- Can prove: every quantum state corresponds to a probability distribution over joint value assignments.
- BUT, don’t know how to efficiently classically parameterize that complete set of probability distributions.

What to do instead?

What are computational implications?

Let $H = \sum_{P \in \mathcal{S}} \alpha_P P$ be observable over noncontextual set $\mathcal{S}$, e.g., $H = \underbrace{\alpha_1 XII + \alpha_2 YII + \alpha_3 ZII}_{\text{anticommute}} + \underbrace{\alpha_4 IZI + \alpha_5 IIZ}_{\text{commute}}$

$\Rightarrow$ H and commuting part of $\mathcal{S}$ share an eigenbasis

$\Rightarrow$ Every eigenvalue of H captured by common eigenvectors of commuting part of $\mathcal{S}$

$\Rightarrow$ Parameterize those common eigenvectors by sets of eigenvalues, e.g., $(IZI \mapsto \pm 1,\ IIZ \mapsto \pm 1)$

$\Rightarrow$ Parameterize anticommuting *generators* by their expectation values (which — recall — satisfy $\sum_i \langle P_i \rangle^2 \leq 1$)

All other operators in set map to products of these

AND exp val of product = product of exp vals when all but one of exp vals are actually eigenvalues!

$$\langle \psi | AB | \psi \rangle = \langle \psi | A \lambda_B | \psi \rangle = \langle \psi | A | \psi \rangle \lambda_B = \langle \psi | A | \psi \rangle \langle \psi | B | \psi \rangle$$

What are computational implications?

Result: every eigenvalue of noncontextual H is included in the set given by

$$\langle H \rangle = \sum_{B \in \mathscr{Z}} \left(\alpha_B + \sum_{i=1}^{N} \alpha_{B,i} r_i \right) \prod_{j \in \mathscr{J}_B} q_j$$

where

$$q_j = \pm 1 \text{ for all } j \text{ and } \sum_{i=1}^{N} r_i^2 \leq 1.$$

Punchline: classical function for eigenvalues of any noncontextual Hamiltonian/observable.

What are computational implications?

Result: every eigenvalue of noncontextual H is included in the set given by

coefficient of BC_i ($C_i = i$th anticommuting generator)

product of eigenvals of commuting generators that form B

$$\langle H \rangle = \sum_{B \in \mathcal{Z}} \left(\alpha_B + \sum_{i=1}^{N} \alpha_{B,i} r_i \right) \prod_{j \in \mathcal{J}_B} q_j$$

element of commuting part

coefficient of B

exp val of C_i

where

$$q_j = \pm 1 \text{ for all } j \text{ and } \sum_{i=1}^{N} r_i^2 \leq 1.$$

Punchline: classical function for eigenvalues of any noncontextual Hamiltonian/observable.

What are computational implications?

So: for noncontextual H, every energy can be written as classical $E(\vec{q}, \vec{r})$, with $\vec{q} \in \{\pm 1\}^M$ and $|\vec{r}| \leq 1$.

Notes:

- Expressed via exp vals; could instead think of $(\vec{q}, \vec{r})$ as parameterizing prob. dists. in noncontextual HVM
- Exp vals ~ marginals of probability distribution
- From exp val side, what makes this classical is *not* that energies can be expressed in terms of exp vals of terms
- It is that you can classically check whether set of exp vals ~ valid quantum state — not possible in general!

Implication:

- Noncontextual Hamiltonian problem is in NP, rather than QMA — $(\vec{q}, \vec{r})$ plus $E(\vec{q}, \vec{r})$, aka set of exp vals, is classical witness

Beyond noncontextual sets

- Ground state energy witness $(\vec{q}, \vec{r}\,)$ for noncontextual $H \leftrightarrow$ subspace of quantum states
- Subspace defined by stabilizers: $\sum_i r_i C_i$ plus $\{q_j G_j\}$

anticommuting generators

commuting generators

"quantum correction"

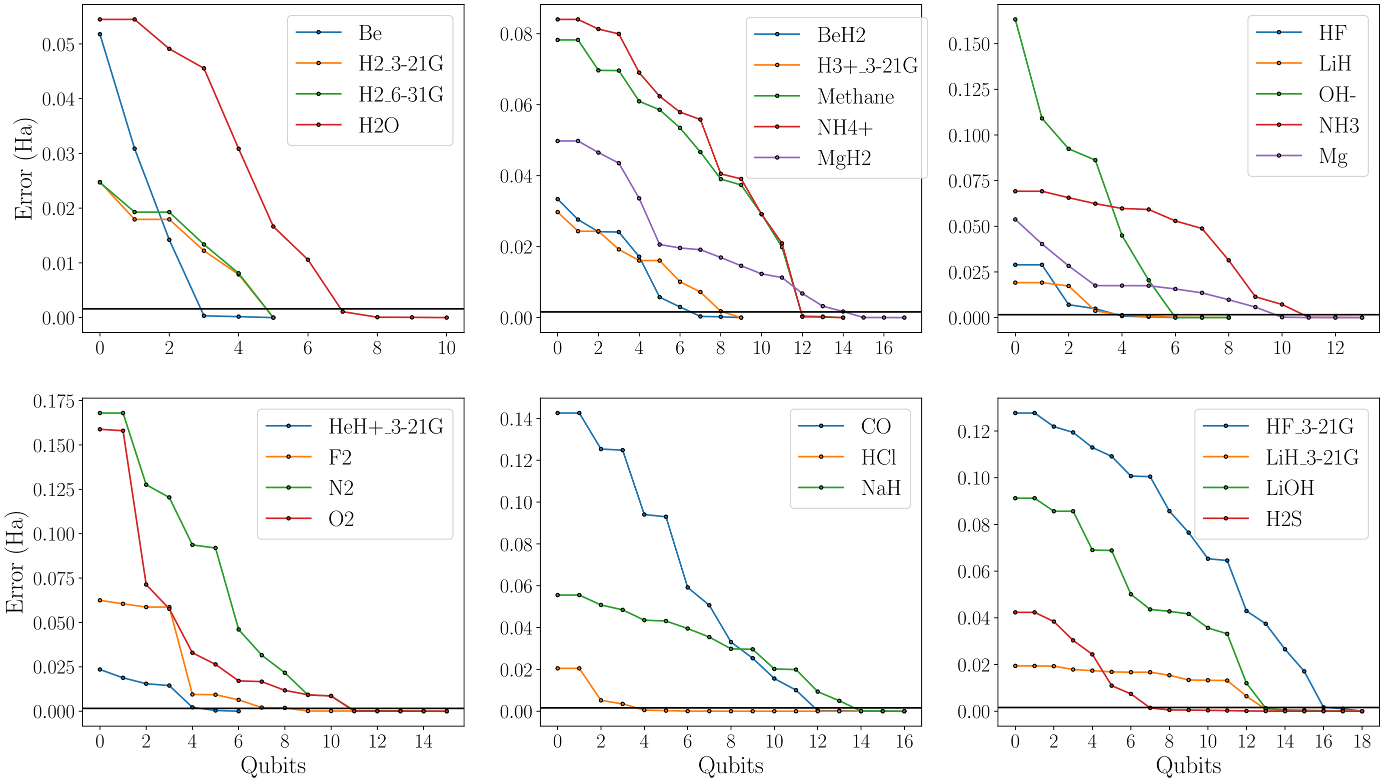
- $\Rightarrow$ If H is contextual, can partition: $H = H_{\text{noncon}} + H_{\text{corr}}$

1. Solve H_{noncon} classically using noncontextual model.
2. Choose number of qubits n_{corr} for quantum correction.
3. Project H_{corr} into subspace defined by $n - n_{\text{corr}}$ of the stabilizers.
4. Solve projected H_{corr} on quantum computer.

“Contextual subspace”

- Previously called this “contextual subspace VQE”
- “Contextual subspace” = subspace in which we solve terms not in noncontextual part
- Not really specific to VQE though…
- Most similar to active spaces: choosing subspace in which to solve “important” part of full correlated problem.
- Also similar to qubit tapering, but in this case, tapering off qubits according to symmetries of noncontextual part of Hamiltonian.

Results for some small molecules



Error vs # qubits used, assuming ideal ground state of projected Hamiltonian in contextual subspace is found. All STO-3G unless specified otherwise.

Thank you!

Main references for this talk:

- William Kirby and Peter Love. *Contextuality test of the nonclassicality of variational quantum eigensolvers*. Phys. Rev. Lett. 123:200501 (2019).
- William Kirby and Peter Love. *Classical simulation of noncontextual Pauli Hamiltonians*. Phys. Rev. A 102:032418 (2020).
- William Kirby, Andrew Tranter, and Peter Love. Contextual subspace variational quantum eigensolver. Quantum 5:456 (2021).

Subsequent work by wonderful collaborators:

- Tim Weaving, Alexis Ralli, William Kirby, Andrew Tranter, Peter Love, and Peter Coveney. *A stabilizer framework for contextual subspace VQE and the noncontextual projection ansatz*. J. Chem. Theory Comput. 19:3:808 (2023).
- Alexis Ralli, Tim Weaving, Andrew Tranter, William Kirby, Peter Love, and Peter Coveney. *Unitary partitioning and the contextual subspace variational quantum eigensolver.* Phys. Rev. Research 5, 013095 (2023).