Exploiting Contextuality in Variational Quantum Eigensolvers

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Outline

1. Contextuality of VQE [KL19]
2. Quasi-quantized (phase-space) model for noncontextual VQE [KL20]
3. Approximation method for contextual VQE [KTL20]

Variational quantum eigensolver

Goal: find ground state energy of

$$H = \sum_{P \in \mathcal{S}} h_P P,$$

for Pauli operators P in some set $\mathcal{S}$.

Method:

1. Main process: on classical computer, minimize

$$E(\vec{\theta}) = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle = \sum_{P \in \mathcal{S}} h_P \langle \psi(\vec{\theta}) | P | \psi(\vec{\theta}) \rangle$$

   for ansatz $|\psi(\vec{\theta})\rangle$.
2. Iteration step: on quantum computer, estimate $\langle P \rangle$ for each $P \in \mathcal{S}$.

Variational quantum eigensolver

Want to understand where "quantumness" appears in this algorithm.

$$H = \sum_{P \in \mathcal{S}} h_P P$$

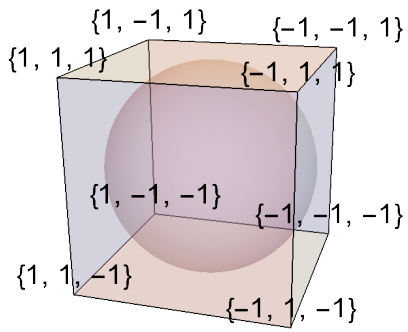
$\Rightarrow$ Focus on $\mathcal{S}$.

Contextuality of Pauli operators

Given $\mathcal{S}$, suppose you want to construct a classical, realistic model (think HVM). This consists of:

1. joint value assignments to $\mathcal{S}$ (the "classical, real" values).
2. probability distributions over the joint value assignments:
   - need to impose uncertainty relation, i.e., restriction on which values can be known simultaneously $\Leftrightarrow$ *quasi-quantization* [Spe16].

For example, suppose $\mathcal{S} = \{X, Y, Z\}$:



value assignments = vertices,
prob. distributions = points in sphere.

Contextuality: when is it possible versus impossible to construct such a model?

Contextuality of Pauli operators

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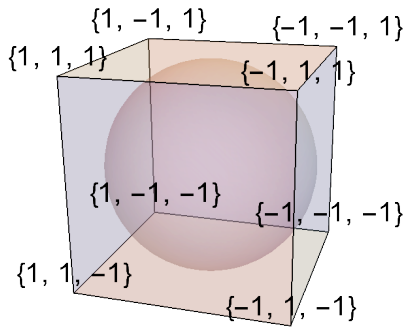

value assignments = vertices,
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Strong contextuality: when is it possible versus impossible to construct the joint value assignments?

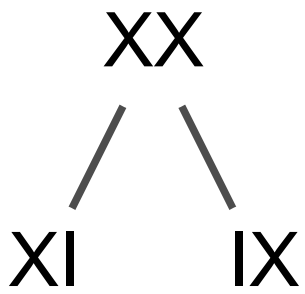
Contextuality of Pauli operators

Focus on joint value assignments (strong contextuality).

Any commuting subset of $\mathcal{S}$ is simultaneously measurable.

$P, Q \in \mathcal{S}$ and $[P, Q] = 0 \quad \Rightarrow \quad$ by measuring P and Q *infer* value assigned to PQ (since joint value assignment interpreted as "real" values for $\mathcal{S}$).

Example. $\mathcal{S} = \{XI, IX\} \quad \Rightarrow \quad$ for assignment $\{\pm 1, \pm 1\}$ to $\mathcal{S}$, can infer assignment to XX:



Contextuality of Pauli operators

Focus on joint value assignments (strong contextuality).

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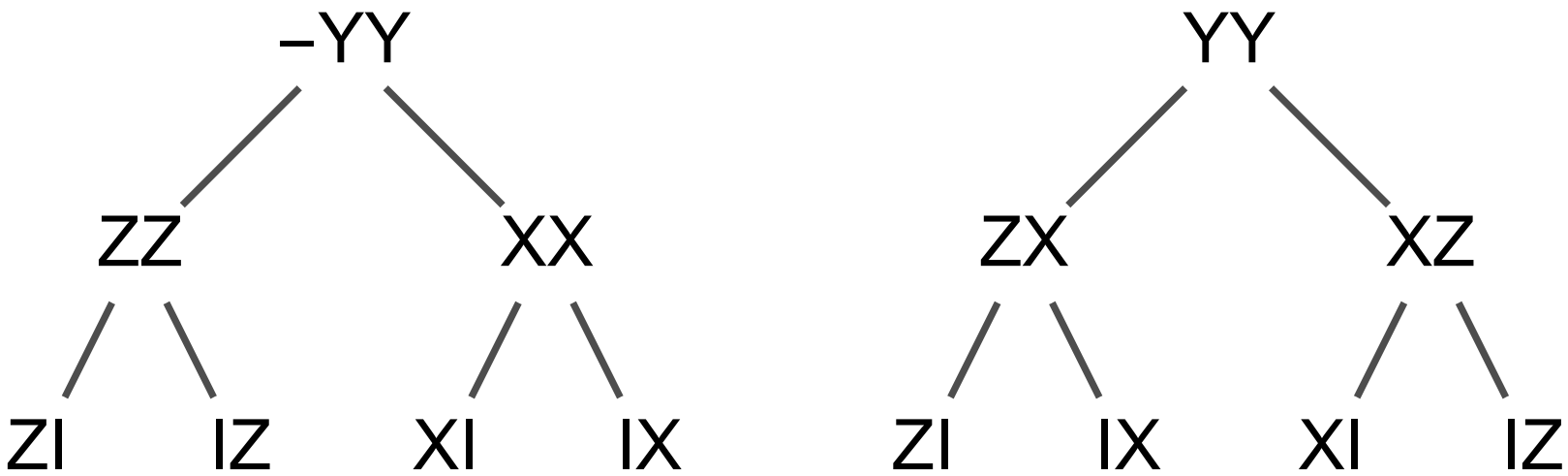
$\mathcal{S}$ is contextual if any joint values necessarily violate some such inference.

Contextuality of Pauli operators

Example: $\mathcal{S} = \{XI, IX, ZI, IZ\}$.



$\Rightarrow$ $\forall$ joint value assignments to $\mathcal{S}$, we infer that YY and $-YY$ have the same value $\Rightarrow$ contradiction! $\Rightarrow$ $\mathcal{S}$ is contextual.

Contextuality of Pauli operators

Result [KL19]. $\mathcal{S}$ is *noncontextual* iff it has the form

$$\mathcal{S} = \mathcal{Z} \cup \mathcal{T} = \mathcal{Z} \cup \mathcal{C}_1 \cup \mathcal{C}_2 \cup \cdots \cup \mathcal{C}_N,$$

where commutation is an equivalence relation on $\mathcal{T}$ ($\mathcal{C}_i$ = equivalence classes), and any $A \in \mathcal{Z}$ commutes with any $B \in \mathcal{S}$.

Definition. Hamiltonian H (VQE instance) is noncontextual iff its set $\mathcal{S}$ of Pauli terms is noncontextual.

Classical simulation of noncontextual Hamiltonians

$\Rightarrow$ can recover Hamiltonian terms by inference on

$$G \cup \{A_1\} \cup \{A_2\} \cup \cdots \cup \{A_N\},$$

where G is independent generating set for $\mathcal{Z}$, and $A_i \in C_i$.

$\Rightarrow$ every noncontextual Hamiltonian has the form:

$$H = \sum_{B \in \overline{G}} \left(h_B B + \sum_{i=1}^{N} h_{B,i} B A_i \right).$$

Allowed probability distributions lead to following sets of expectation values:

$$\langle G_j \rangle = q_j = \pm 1, \quad \langle A_i \rangle = r_i$$

for $|\vec{r}| = 1$. Can prove these are enough to generate all possible expectation values of Hamiltonian.

Classical simulation of noncontextual Hamiltonians

Given any noncontextual H...

Result [KL20]. For parameters $q_j = \pm 1$ and $|\vec{r}| = 1$.

$$\langle H \rangle_{(\vec{q},\vec{r})} = \sum_{B \in \overline{G}} \left(h_B + \sum_{i=1}^{N} h_{B,i} r_i \right) \prod_{j \in \mathcal{J}_B} q_j,$$

for $\mathcal{J}_B$ s.t. $B = \prod_{j \in \mathcal{J}_B} G_j$.

Classical objective function of at most $2n + 1$ real parameters.

Immediate consequences:

1. "dequantization" of noncontextual VQE.
2. noncontextual Hamiltonian problem is in NP.

Hybrid simulation of contextual Hamiltonians

Given any arbitrary H, can partition:

$$H = H_{\text{n.c.}} + H_{\text{c.}},$$

where $H_{\text{n.c.}}$ is noncontextual and as large as possible.

Noncontextual ground state $(\vec{q}, \vec{r})_0$ of $H_{\text{n.c.}}$ corresponds to subspace of quantum states: common eigenspace of G_j (eigenvalues q_j) and

$$\mathcal{A} \equiv \sum_{i=1}^{N} r_i A_i \qquad \text{(eigenvalue } +1\text{)}.$$

On quantum computer, can minimize expectation value of $H_{\text{c.}}$ within this subspace to obtain correction to noncontextual ground state energy.

Contextual Subspace VQE (CS-VQE)

Result [KTL20].

$$H = H_{\text{n.c.}} + H_{\text{c.}}$$

$\langle H_{\text{n.c.}} \rangle$ is determined classically, $\langle H_{\text{c.}} \rangle$ is determined quantumly.

Each "stabilizer" G_j and $\mathcal{A}$ removes one qubit's worth of freedom from the quantum search space, so $H_{\text{c.}}$ becomes Hamiltonian on $n - 1 - |G|$ qubits.

Can we use more quantum resources to improve accuracy?

Yes. Drop some of the G_j (and inferred terms) from noncontextual part, simulating them instead on the quantum computer.

Applying Contextual Subspace VQE to molecules

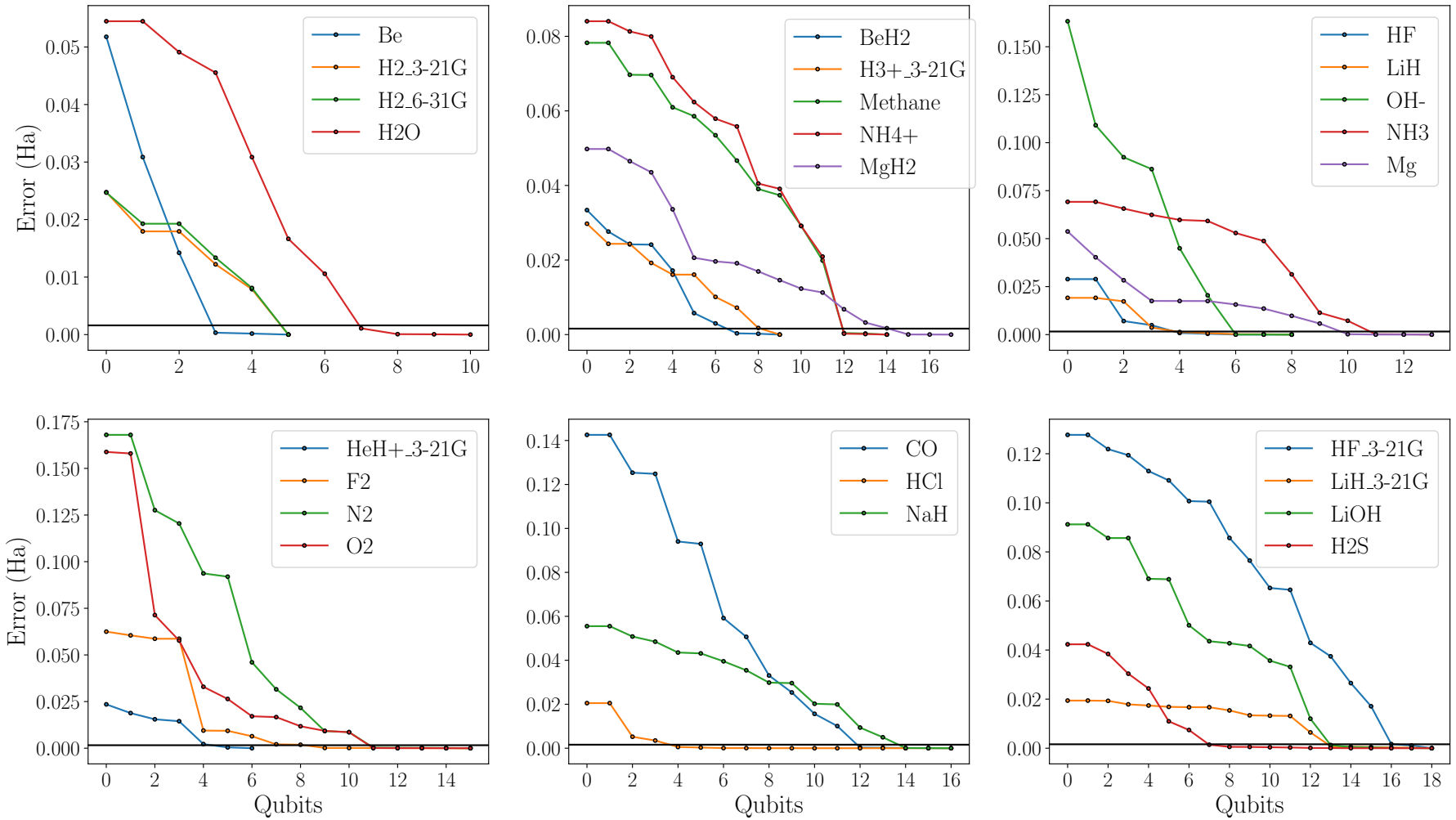


Figure: CS-VQE approximation errors versus number of qubits used on the quantum computer, for tapered Hamiltonians. Black line is chemical accuracy.

Thank you! Any questions?


William M. Kirby and Peter J. Love. Contextuality test of the nonclassicality of variational quantum eigensolvers. *Phys. Rev. Lett.*, 123:200501, Nov 2019.


William M. Kirby and Peter J. Love. Classical simulation of noncontextual pauli hamiltonians. *Phys. Rev. A*, 102:032418, Sep 2020.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Robert W. Spekkens. *Quasi-Quantization: Classical Statistical Theories with an Epistemic Restriction*, pages 83–135. Springer Netherlands, Dordrecht, 2016.

Code: `https://github.com/wmkirby1/ContextualSubspaceVQE`

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