Contextual Subspace Variational Quantum Eigensolver

Will Kirby[1], Andrew Tranter[1,2], Alexis Ralli[3], Tim Weaving[3], Peter Coveney[3], and Peter Love[1,4]

[1]Department of Physics and Astronomy, Tufts University, Medford, MA 02155

[2]Cambridge Quantum Computing, Cambridge, CB2 1UB, United Kingdom

[3]Centre for Computational Science, Department of Chemistry, University College London, WC1H 0AJ, United Kingdom [4]Computational Science Initiative, Brookhaven National Laboratory, Upton, NY 11973

Harvard Mathematical Picture Language Seminar

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STANDARD CANDLES

RR LYRAE
RED SHIFT
CEPHEID
VARIABLES
PARALLAX
TYPE-II SUPERNOVAE
GRAVITATIONAL WAVES

. 3-SAT

. MAX-CUT

FACTORING

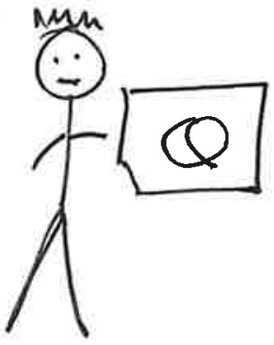
.

. QUANTUM DYNAMICS

. LOCAL HAMILTONIAN

. GRAPH ISOMORPHISM

ENTANGLEMENT
CONTEXTUALITY
DISCORD
MAGIC
NEGATIVITY



T-COUNT
LOCALITY
CONDITION #
SPARSITY

?

NO STANDARD CANDLES

BUT

FOUNDATIONS OF QM SHOULD HELP DISTINGUISH QUANTUM FROM CLASSICAL

Outline

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:

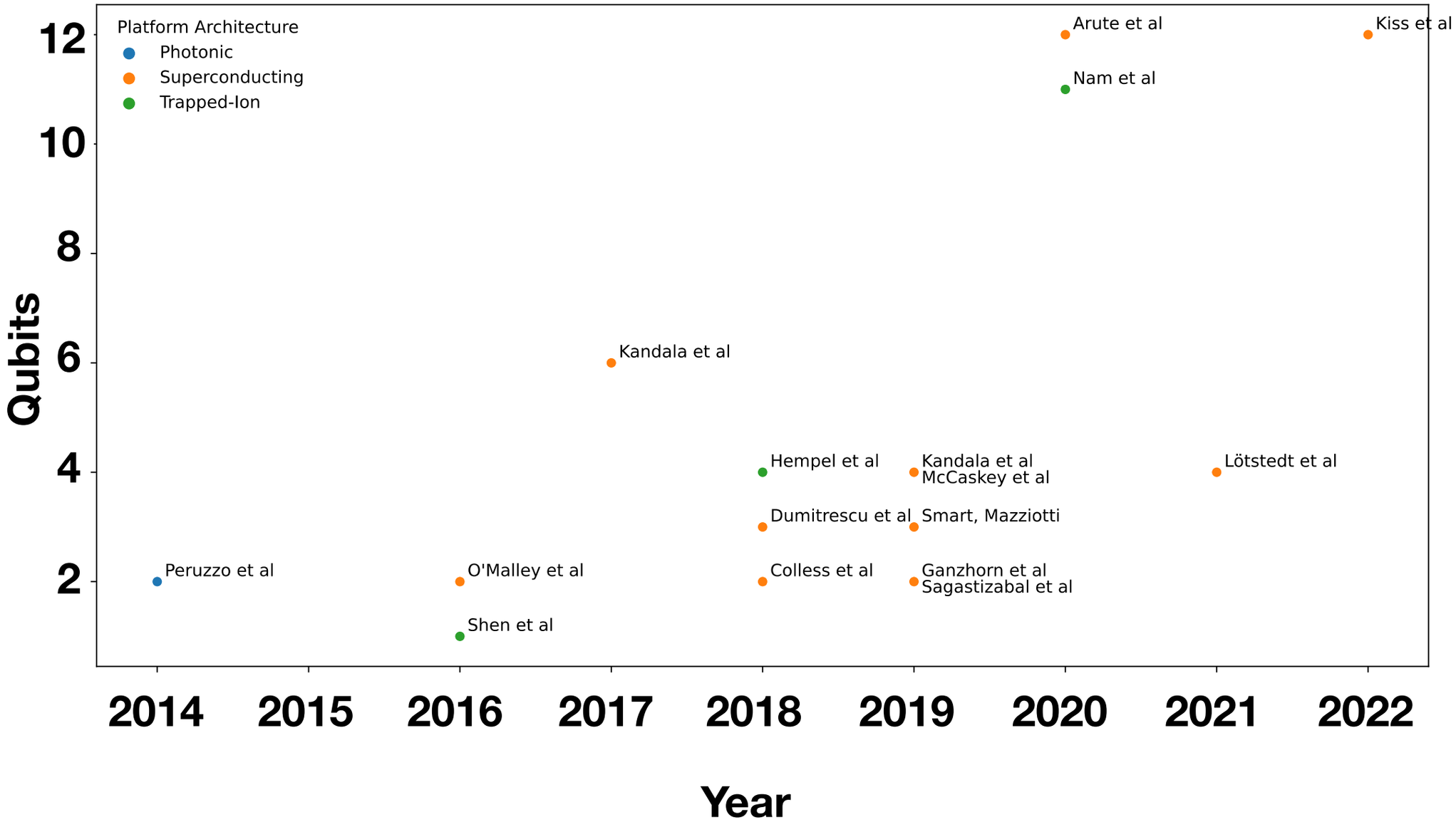
1. Main process: on classical computer, minimize

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

   for ansatz $|\psi(\vec{\theta})\rangle$.

2. Iteration step: on quantum computer, estimate $\langle P \rangle$ for each $P \in \mathcal{S}$.

Experimental implementations of VQE



Molecules Examined:

- HeH^+ (2)
- Deuteron
- H_2 (7)
- H_3
- H_6
- H_8
- H_{10}
- H_{12}
- LiH (3)
- BeH_2
- NaH
- KH
- RbH
- H_2O
- CO_2
- Li
- Heisenberg Model

Outline

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.

Two Obstacles:

1) Uncertainty principle: cannot assign definite values to non commuting operators

2) Strong measurement contextuality: cannot pre-assign values to commuting operators without contradiction

Solve 1) by imposing an uncertainty relation on the epistemic states (probability distributions) of the classical model (a "quasi-quantized model")

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

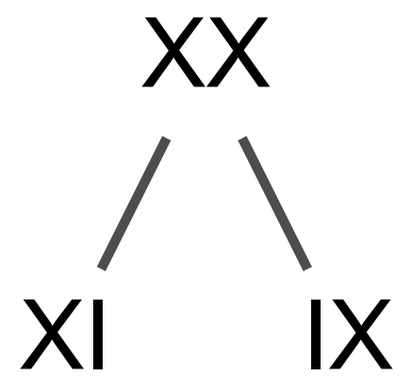
Contextuality of Pauli operators

Focus on joint value assignments.

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 $\mathcal{S}$).

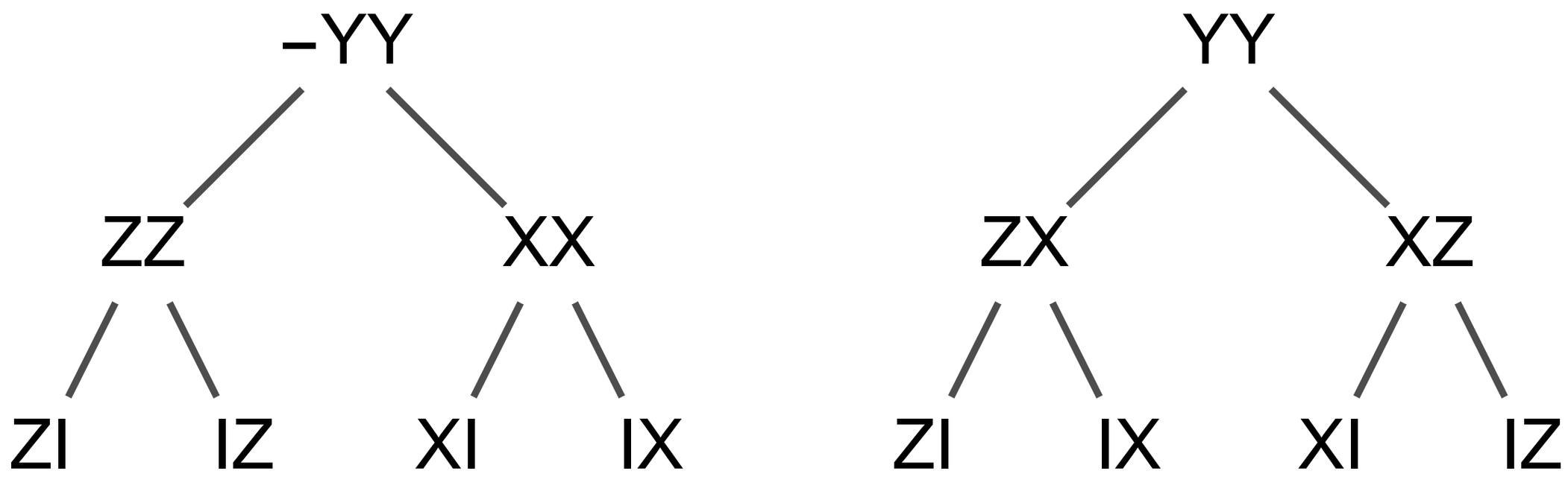
Example. $\mathcal{S} = \{XI, IX\} \quad \Rightarrow \quad$ for assignment $\{\pm 1, \pm 1\}$ to $\mathcal{S}$, can infer assignment to XX:



$\mathcal{S}$ 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 $B \in \mathcal{S}$.

Special cases of noncontextual sets:

1. any commuting set.
2. any anticommuting set.
3. any set in which commutation is an equivalence relation (includes cases 1 and 2): for example, $\{(XI, XZ), (YI, YZ), (ZI, ZZ)\}$.

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

Does a VQE experiment admit a classical interpretation of measurement?

Citation:	System:	Contextual?	CD_0	$\lvert\mathcal{S}\rvert$
Dumitrescu *et al.* [22]	Deuteron	No	0	—
Kandala *et al.* [17]	H_2	No	0	4
O'Malley *et al.* [13]	H_2	No	0	5
Hempel *et al.* [18]	H_2 (BK)	No	0	5
Hempel *et al.* [18]	H_2 (JW)	No	0	14
Colless *et al.* [19]	H_2	No	0	5
Kokail *et al.* [23]	Schwinger Model	Yes	$\sim$0.16	231
Nam *et al.* [20]	H_2O	Yes	0.27	22
Hempel *et al.* [18]	LiH	Yes	0.33	12
Peruzzo *et al.* [11]	HeH^+	Yes	0.38	8
Kandala *et al.* [17]	BeH	Yes	$\sim$0.74	164
Kandala *et al.* [17, 21]	LiH	Yes	$\sim$0.77	99

TABLE I. Evaluation of contextuality in VQE experiments. CD_0 is the minimum number of terms we must remove from the Hamiltonian to reach a noncontextual set, as a fraction of the total number of terms ($|\mathcal{S}|$). In [22], $|\mathcal{S}|$ varies.

Kirby, William M., and Peter J. Love. "Contextuality test of the nonclassicality of variational quantum eigensolvers." Physical Review Letters 123.20 (2019): 200501.

Outline

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 $|\vec{r}| = 1$.

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

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.

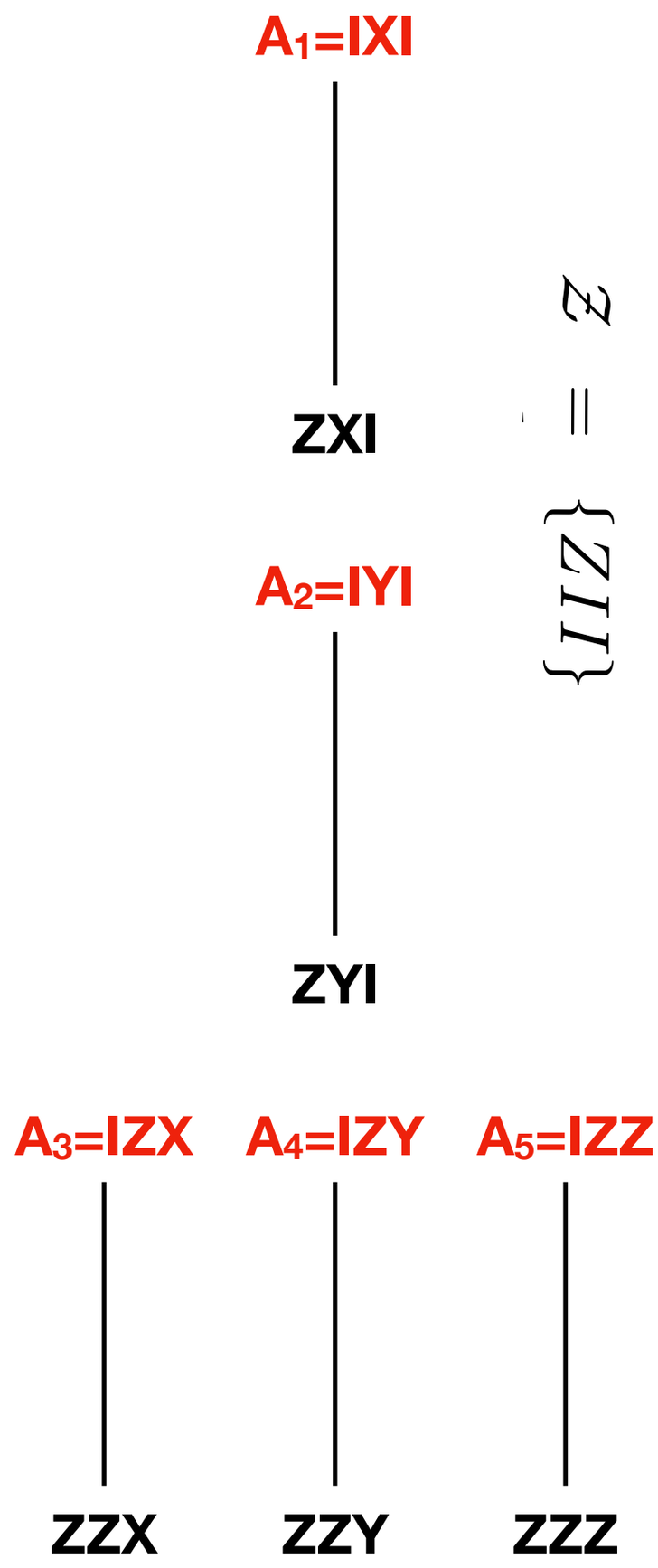
2.4 Example

As an example, we construct a Hamiltonian for which most of the terms are included in the non-contextual part. Let $\mathcal{S} = \mathcal{S}_{\rm nc} \cup \mathcal{S}_{\rm c}$, where

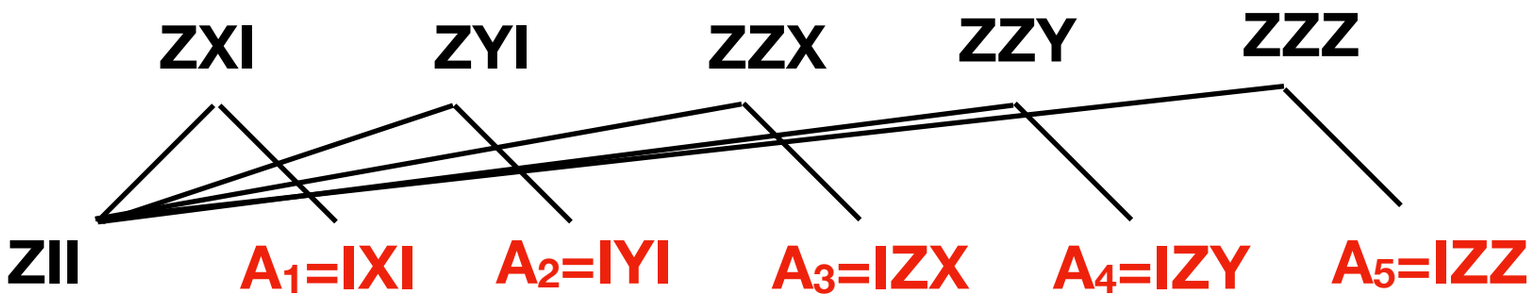
$$\begin{aligned}\mathcal{S}_{\rm nc} = \{&ZII, IXI, IYI, IZX, IZY, IZZ,\\ &ZXI, ZYI, ZZX, ZZY, ZZZ\},\\ \mathcal{S}_{\rm c} = \{&IIX, IIY, IIZ\}.\end{aligned} \tag{13}$$

The set of terms $\mathcal{S}_{\rm nc}$ is noncontextual, partitioning into $\mathcal{Z} = \{ZII\}$ (recall that $\mathcal{Z}$ is the set of terms that commute with all others), and five cliques, $\{IXI, ZXI\}$, $\{IYI, ZYI\}$, $\{IZX, ZZX\}$, $\{IZY, ZZY\}$, and $\{IZZ, ZZZ\}$. Thus we may choose

$$\begin{aligned} &A_1 = IXI,\ A_2 = IYI,\ A_3 = IZX, \\ &A_4 = IZY,\ A_5 = IZZ. \end{aligned} \tag{14}$$



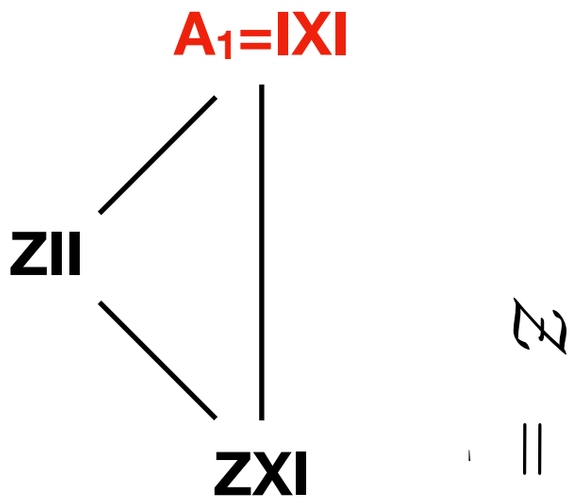
Inference on the NC Hamiltonian S



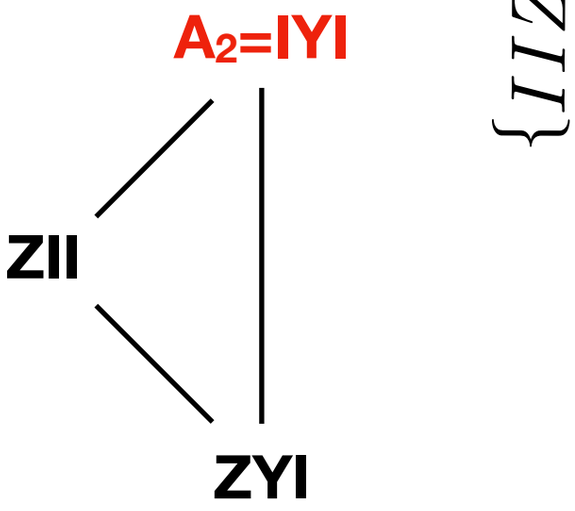
I assign a value to ZII, choosing a symmetry sector.

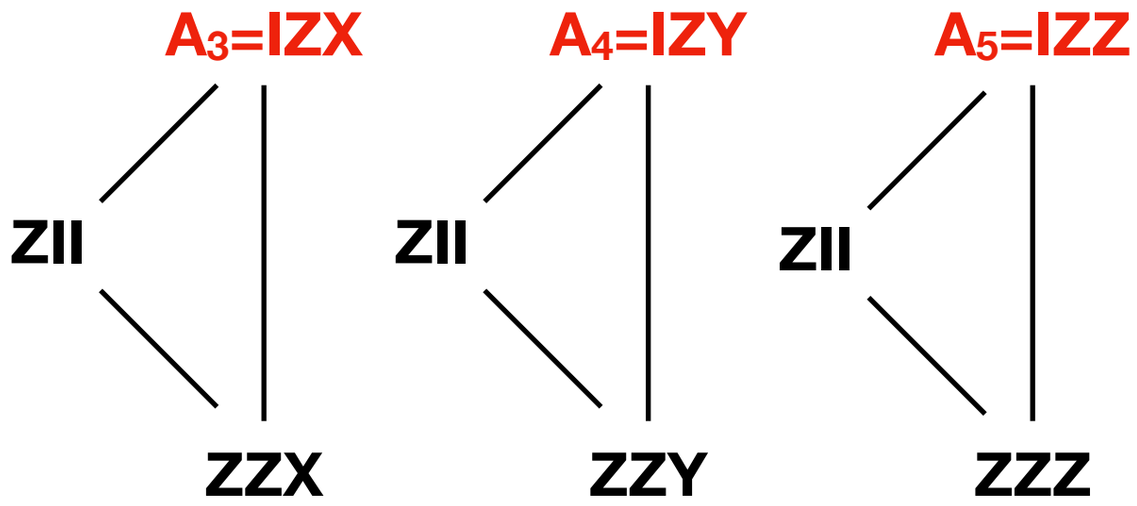
I assign each of A1, A2, A3, A4, A5

From the A's and ZII we can infer assignments to all operators



$\Xi = \{ZII\}$



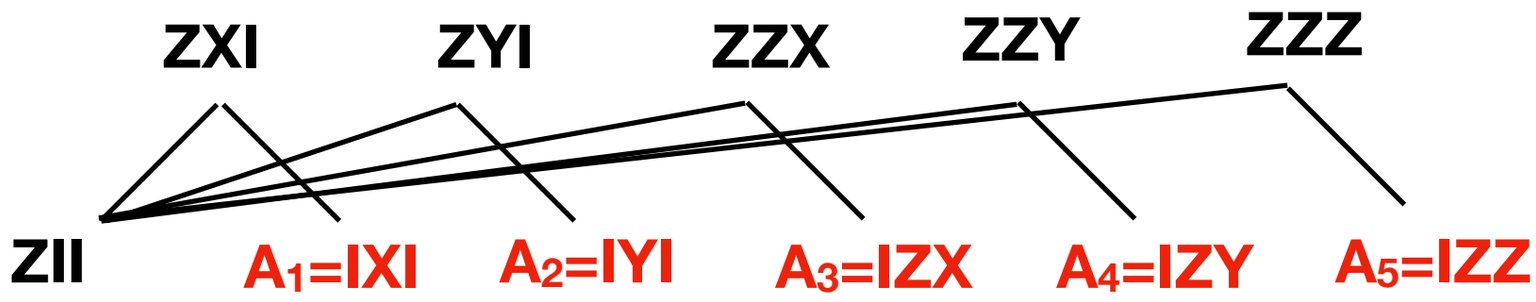


Inference on the NC Hamiltonian S

ZII commutes with everything and so can be assigned +1, -1 without contradicting the uncertainty principle.

The A's anticommute so the simultaneous assignment of these operators violates the uncertainty principle.

We must reimpose the uncertainty principle by specifying a probability distribution over assignments of the A's.



Epistemic states

Probability distribution over assignments of c_i to A_i and g_i to G_i given q_j and **r**

$$P_{(\vec{q},\vec{r})}(c_1, \ldots, c_N, g_1, g_2, \ldots) = \left(\prod_{j=1}^{|G|} \delta_{g_j, q_j} \right) \prod_{i=1}^{N} \frac{1}{2} |c_i + r_i|.$$

Selects correct symmetry sector

Enforces correct expectation values of A

Equivalent to specifying epistemic state by

$$\langle G_j \rangle = q_j = \pm 1, \quad \langle A_i \rangle = r_i, \quad |\vec{r}| = 1.$$

Noncontextual approximation

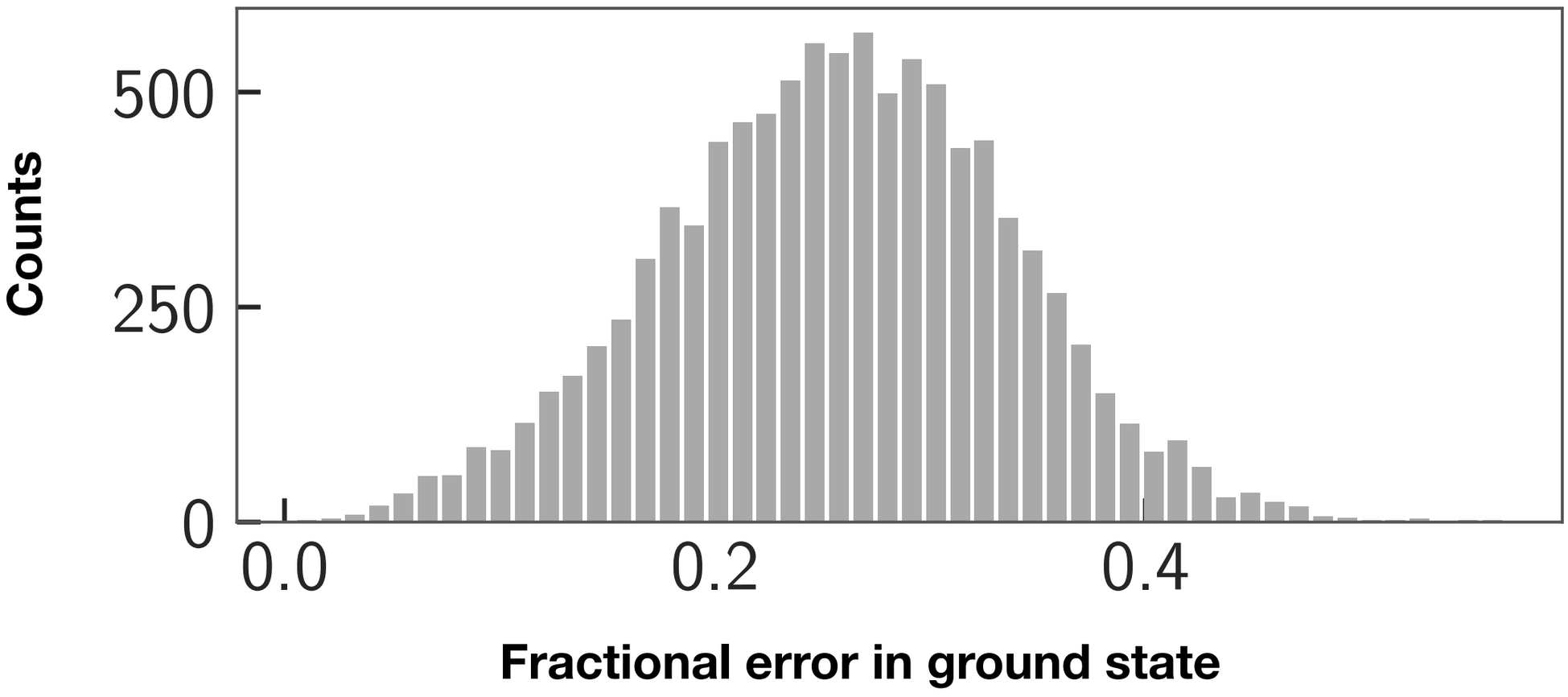
Returning to our example:

$$\mathcal{S}_{\rm nc} = \{ZII, IXI, IYI, IZX, IZY, IZZ, ZXI, ZYI, ZZX, ZZY, ZZZ\},$$

$$\mathcal{S}_{\rm c} = \{IIX, IIY, IIZ\}.$$

Look at 10000 full Hamiltonians with coefficients uniformly random in [-1,1]

Plot fractional error of non-contextual approximation



Does a VQE experiment admit a noncontextual hidden variable theory that can achieve the same accuracy?

Citation	System	n	$\lvert\mathcal{S}_{\text{full}}\rvert$	$\lvert\mathcal{S}_{\text{noncon}}\rvert$	$\lvert\mathcal{R}\rvert$	ϵ_{noncon}	ϵ_{diag}	ϵ_{expt}	Expt. outperforms noncontextual?
Peruzzo *et al.*, 2014 [2]	HeH^+	2	9	5	3	0.21	4.1	4.1	No
Hempel *et al.*, 2018 [11]	LiH	3	13	9	4	0.56	0.56	∼80	No
Kandala *et al.*, 2017 [10]	LiH	4	99	23	5	4.2	9.3	∼30	No
Kandala *et al.*, 2017 [10]	BeH_2	6	164	42	7	156	266	∼90	Yes

TABLE I. Contextual VQE experiments, as approximated by noncontextual and diagonal Hamiltonians. n is the number of qubits. $|\mathcal{S}_{\text{full}}|$ is the number of terms in the full Hamiltonian, $|\mathcal{S}_{\text{noncon}}|$ is the number of terms in the noncontextual sub-Hamiltonian, and $|\mathcal{R}|$ is the number of parameters in an epistemic state (which is upper bounded by $2n+1$ for n qubits). ϵ_{noncon} is the error in the noncontextual approximation, ϵ_{diag} is the error obtained by only keeping the diagonal terms in the Hamiltonian, and ϵ_{expt} is the error in the VQE experiment. Errors are in units of chemical accuracy, 0.0016Ha. Experimental errors preceded by $\sim$ were estimated from figures.

Kirby, William M., and Peter J. Love. "Classical simulation of noncontextual Pauli Hamiltonians." Physical Review A 102.3 (2020): 032418.

Outline

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 [KTL21].

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

$\langle H_{\text{n.c.}} \rangle$ 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_js (and inferred terms) from noncontextual part, simulating them instead on the quantum computer.

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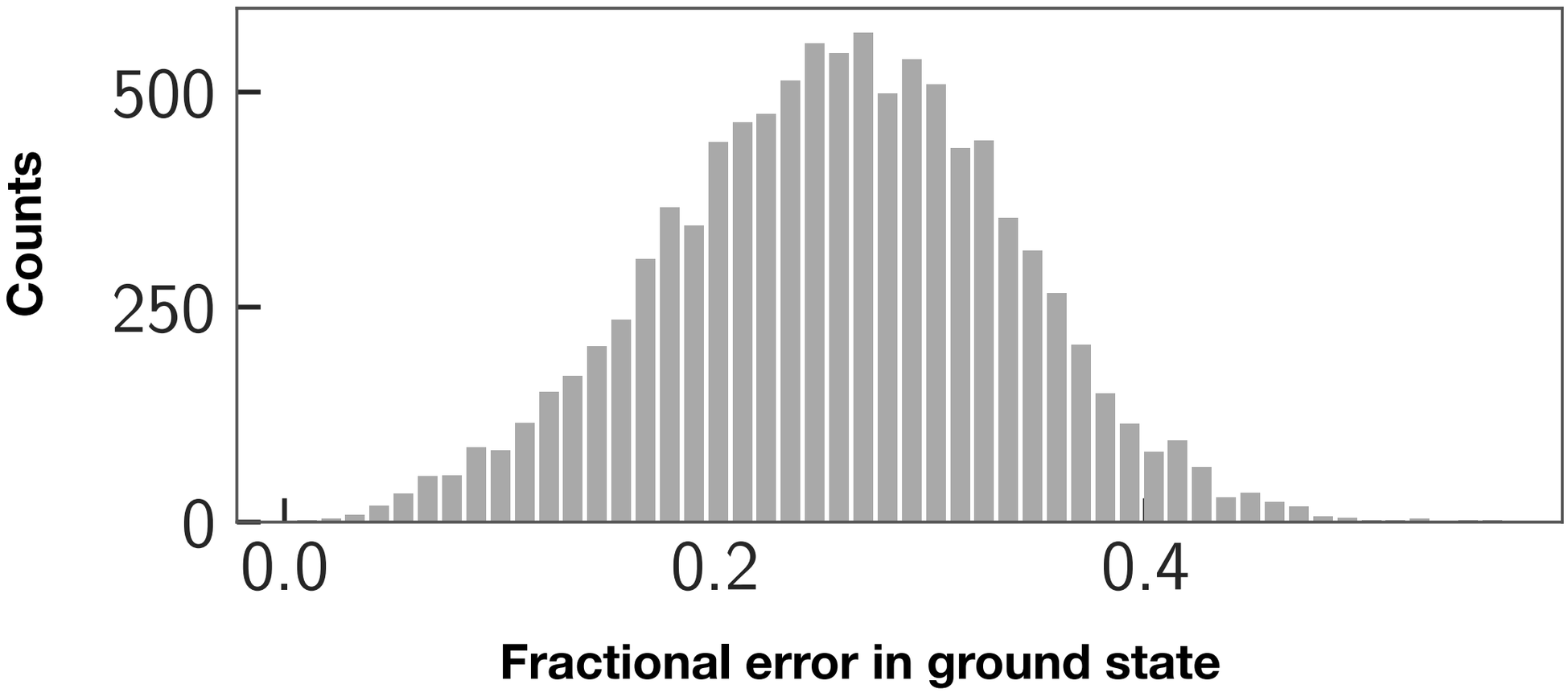
$$\mathcal{S}_{\rm c} = \{IIX, IIY, IIZ\}.$$

Look at 10000 full Hamiltonians with coefficients uniformly random in [-1,1]

Plot fractional error of non-contextual approximation



Contextual correction

$$\mathcal{S}_{\rm nc} = \{ZII, IXI, IYI, IZX, IZY, IZZ,$$
$$ZXI, ZYI, ZZX, ZZY, ZZZ\},$$
$$\mathcal{S}_{\rm c} = \{IIX, IIY, IIZ\}.$$

$$H'_{\rm c} = H_{\rm c} = h_{IIX} IIX + h_{IIY} IIY + h_{IIZ} IIZ$$

Can remove one qubit per noncontextual generator

$$H'_{\rm c}|_{\mathcal{H}_2} = H_{\rm c} = h_{IIX} IX + h_{IIY} IY + h_{IIZ} IZ. \quad (16)$$

We also have

$$\mathcal{A}' = \mathcal{A} = r_1 A_1 + r_2 A_2 + r_3 A_3 + r_4 A_4 + r_5 A_5$$

$$\mathcal{A}'|_{\mathcal{H}_2} = r_1 XI + r_2 YI + r_3 ZX + r_4 ZY + r_5 ZZ,$$

$$D_{\mathcal{A}'} \mathcal{A}'|_2 D^\dagger_{\mathcal{A}'} = ZI; \quad (19)$$

in this case, for an ansatz we may prepare any state whose value is $|0\rangle$ for the first qubit in $\mathcal{H}_2$, and then apply $D^\dagger_{\mathcal{A}'}$ to this state.

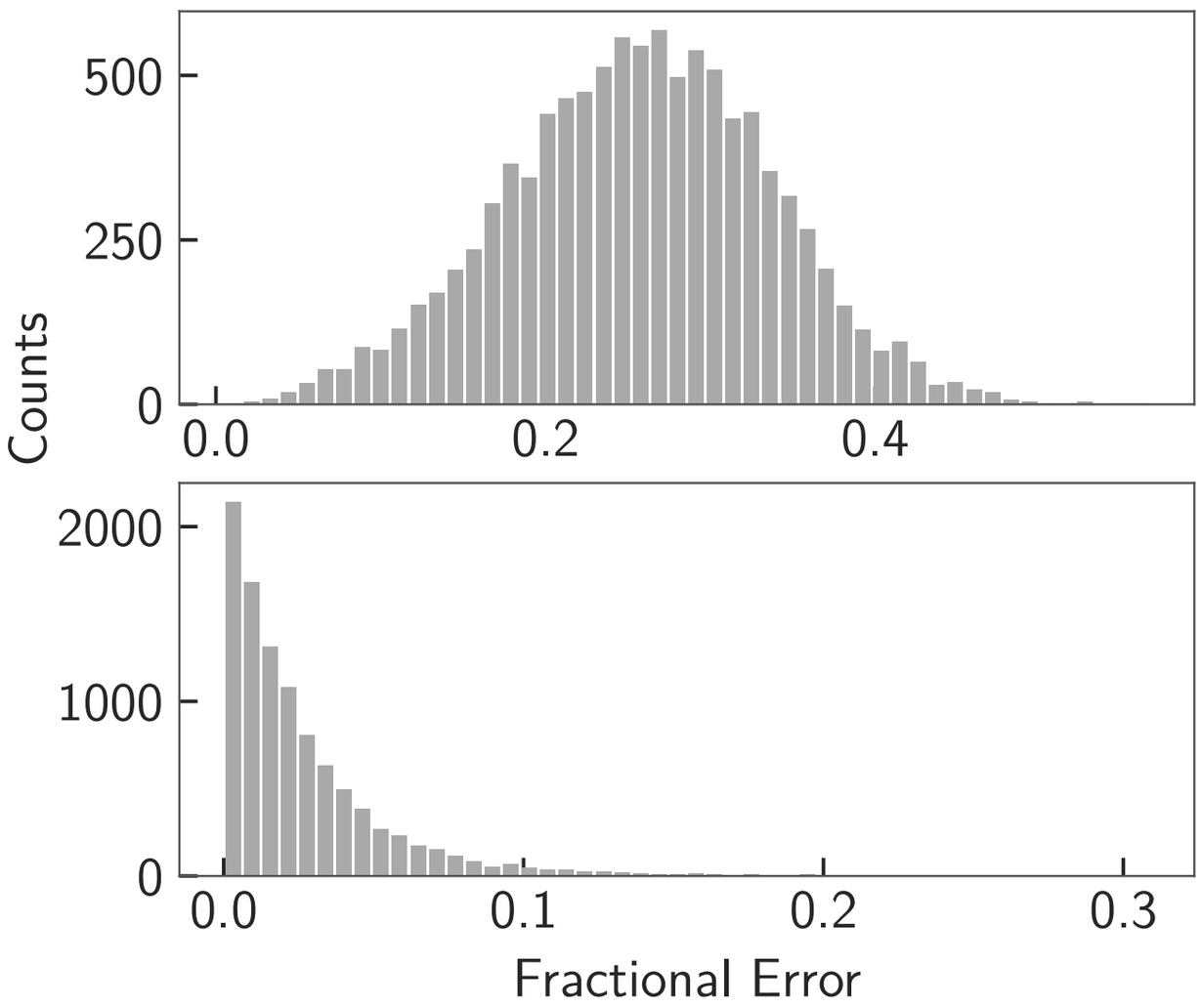


Figure 1: Comparison of fractional errors in the noncontextual approximation of the ground state energy (upper plot), and in the noncontextual approximation with quantum correction (lower plot). The histogram points were generated by 10000 Hamiltonians with terms (13) and uniformly random coefficients in $[-1, 1]$. The mean fractional error without quantum correction is 0.257, and the mean fractional error with quantum correction is 0.0268.

Applying Contextual Subspace VQE to molecules

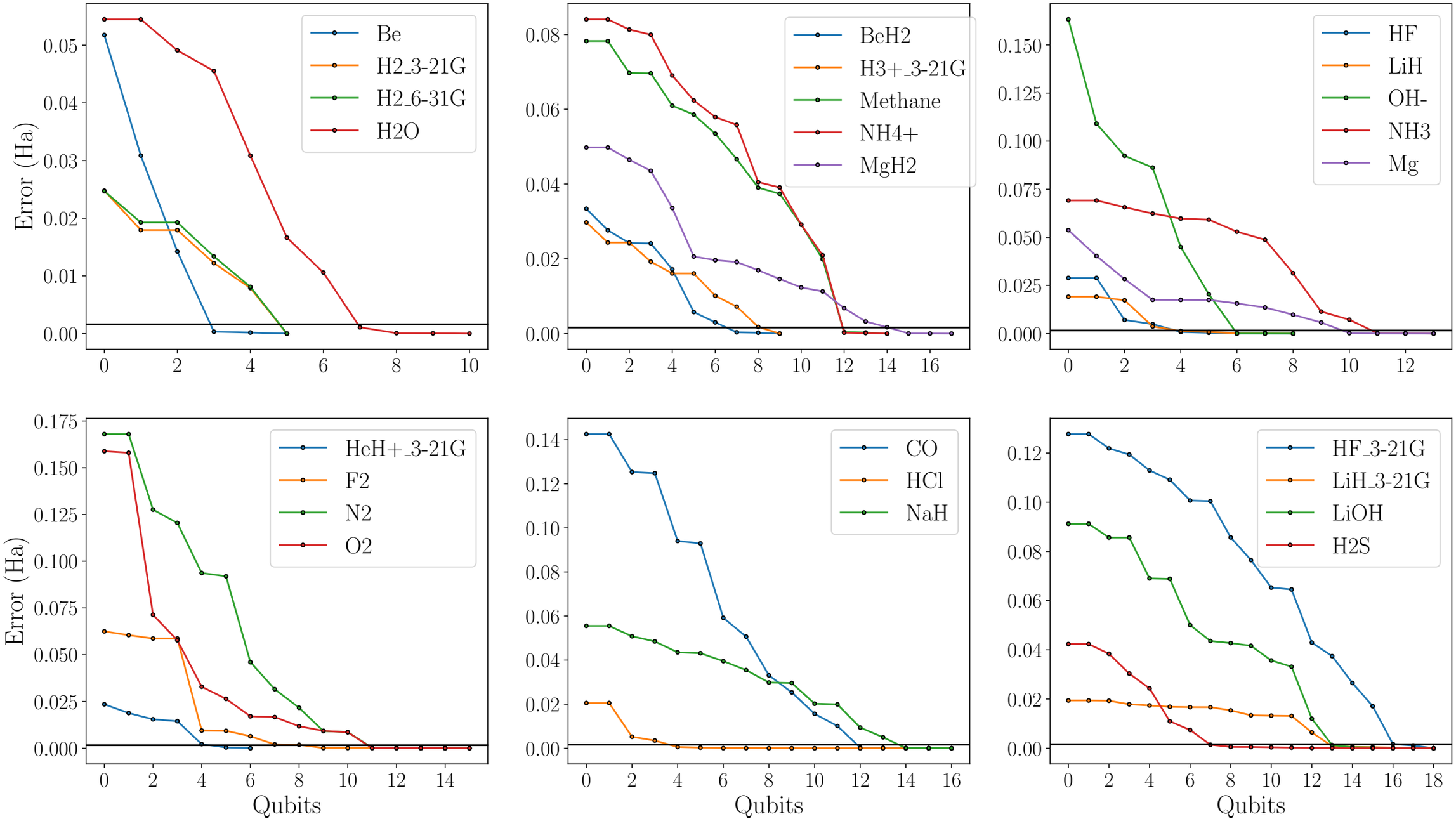
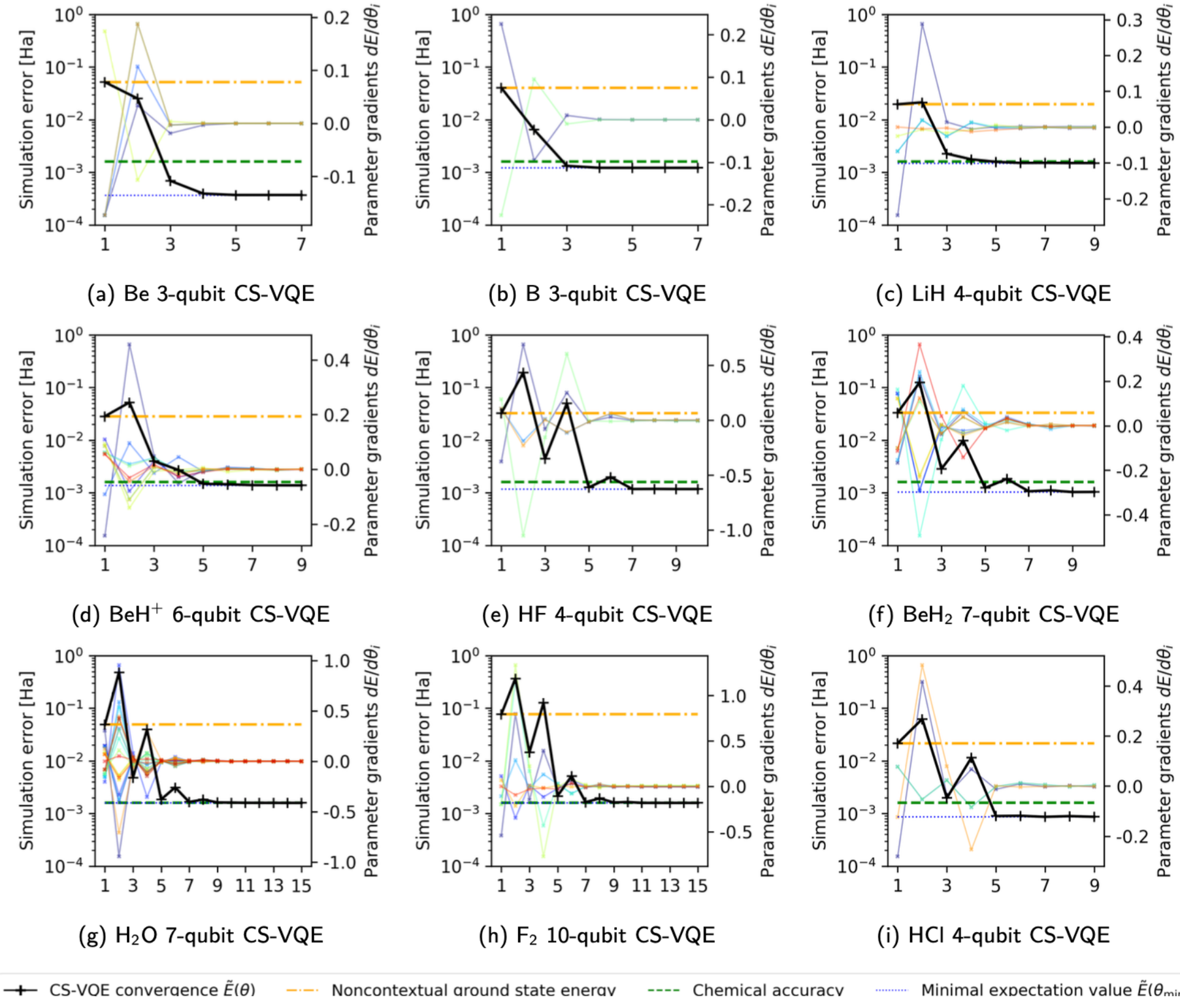


Figure: CS-VQE approximation errors versus number of qubits used on the quantum computer, for tapered Hamiltonians. Black line is chemical accuracy.

Applying CS-VQE to molecules [WRK+22]



(a) Be 3-qubit CS-VQE

(b) B 3-qubit CS-VQE

(c) LiH 4-qubit CS-VQE

(d) BeH^+ 6-qubit CS-VQE

(e) HF 4-qubit CS-VQE

(f) BeH_2 7-qubit CS-VQE

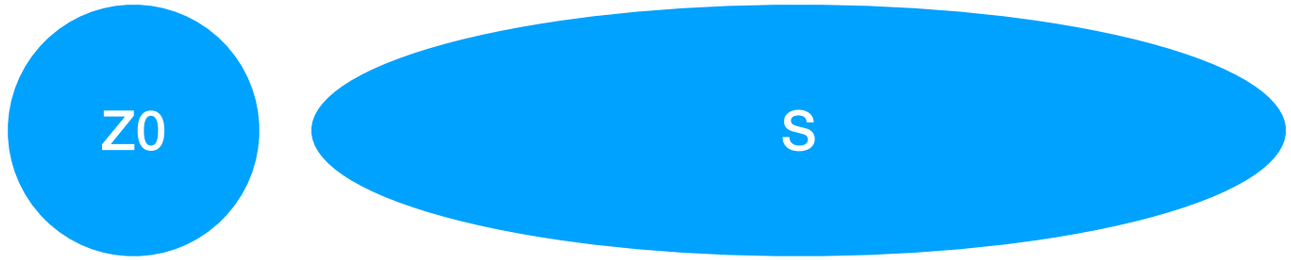
(g) H_2O 7-qubit CS-VQE

(h) F_2 10-qubit CS-VQE

(i) HCl 4-qubit CS-VQE

Given arbitrary Pauli Hamiltonian H how do we split into H_{nc} and H_c?

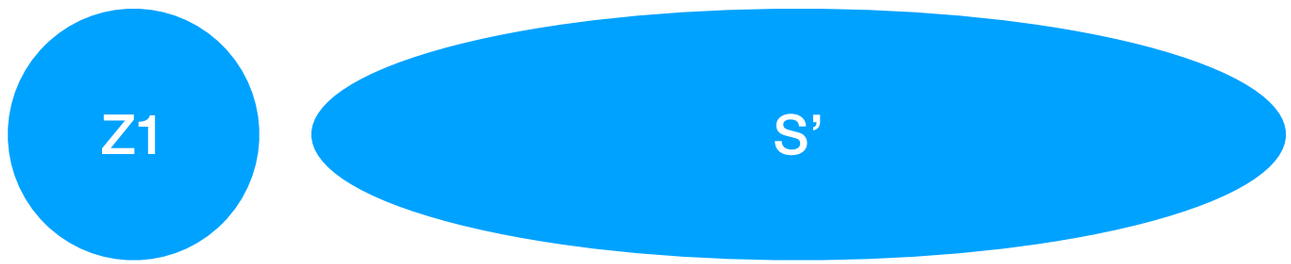
Original H



Assume empty

Now remove some terms from S

H'



New H could become more symmetric

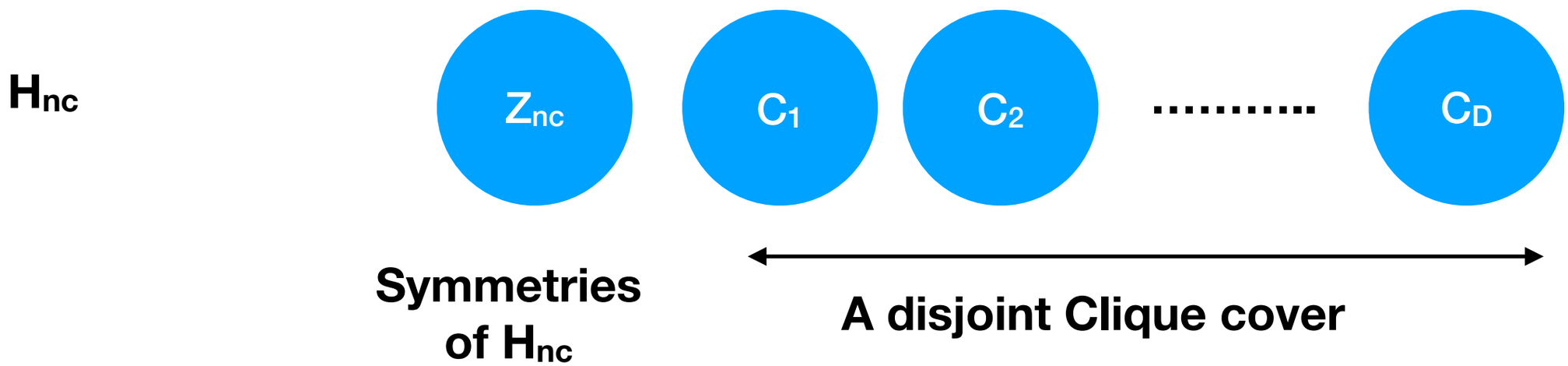
We want:

H_{nc}

Symmetries of Hnc

A disjoint Clique cover

Given arbitrary Pauli Hamiltonian H how do we split into Hnc and Hc?



Easier to state problem in terms of compatibility graph of H: edges between terms that commute

Finding a subgraph with this structure is already hard - Max Clique cover is NP complete [JSW].

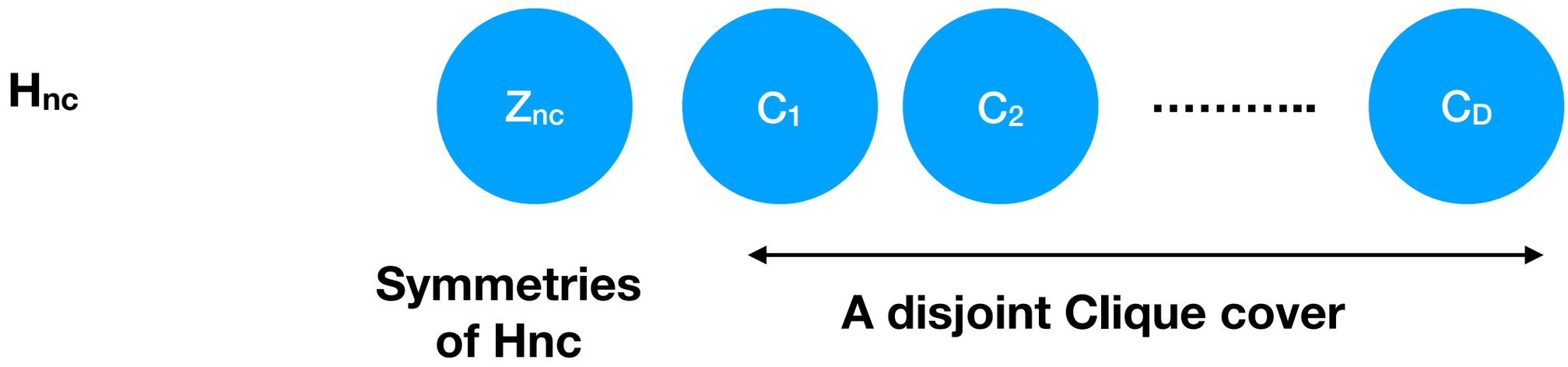
But we want more! Want H_{nc} ground state to well approximate H ground state.

First: discuss graph problem (gives us an idea of hardness)

Second discuss heuristics for Hamiltonian approximation

[JSW] K. Jansen, P. Scheffler, and G. Woeginger, Maximum Covering with D Cliques in FCT, Lecture Notes in Computer Science, Vol. 710 (1993) pp. 319–328.

Disjoint union of Cliques



Finding a Hamiltonian with this structure is already hard - DISJOINT UNION OF CLIQUES is NP complete [JSW].

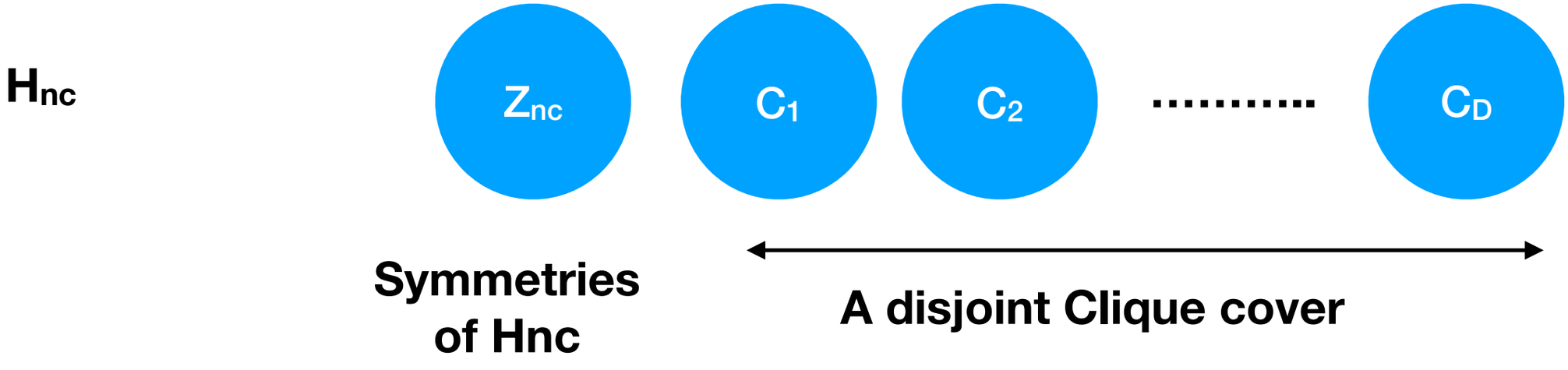
DISJOINT UNION OF CLIQUES (DUC) Given a finite undirected graph G=(V, E) and two positive integers D, B<=|V|, decide whether there are D pairwise disjoint cliques C1….CD such that the cliques cover at least B vertices.

If D=1, only one clique, this is the CLIQUE problem - NP-complete (Johnson)

If B=|V| this is the PARTITION INTO CLIQUES problem - NP-complete (Johnson)

But let's look in a bit more detail…..

Given arbitrary Pauli Hamiltonian H how do we split into Hnc and Hc?



But we want more! Want H_{nc} ground state to well approximate H ground state.

Done: Try various Heuristics and compare them numerically

To do: try to prove some performance bounds on the heuristics (would be nice)

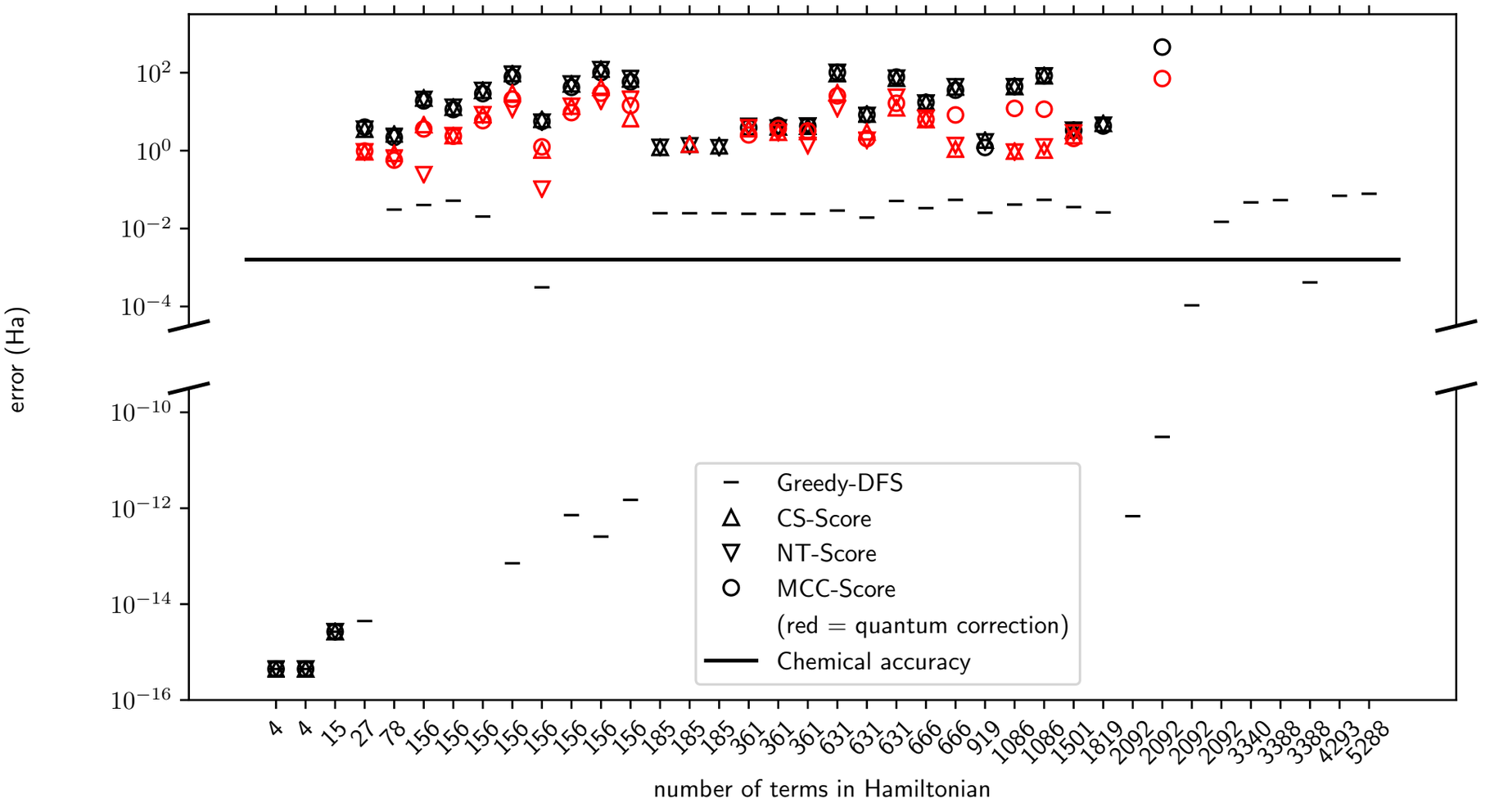
To do: try to prove restrictions on complexity for various classes of graphs (would be nice)

Heuristics

Want to keep terms that contribute a lot to ground state energy (large expectation values) and discard terms that do not. Two kinds of approximation:

1) **Use magnitude of coefficient as a proxy for contribution (done)**
2) **Use classical methods to estimate magnitudes (not done)**

Results on 38 electronic structure Hamiltonians



Why is DFS best?

Hartree-Fock is pretty good - small correlation energy means diagonal terms dominate in terms of coefficient magnitude.

DFS always includes all the diagonal terms.

How many off diagonal terms can you add and still be noncontextual?

Start with the highest coefficient off diagonal term C21

Diagonal terms C21 commutes with

Clique {C21}

Clique of terms C21 anticommutes with

Why is DFS best?

Diagonal terms C21 commutes with

Clique {C21}

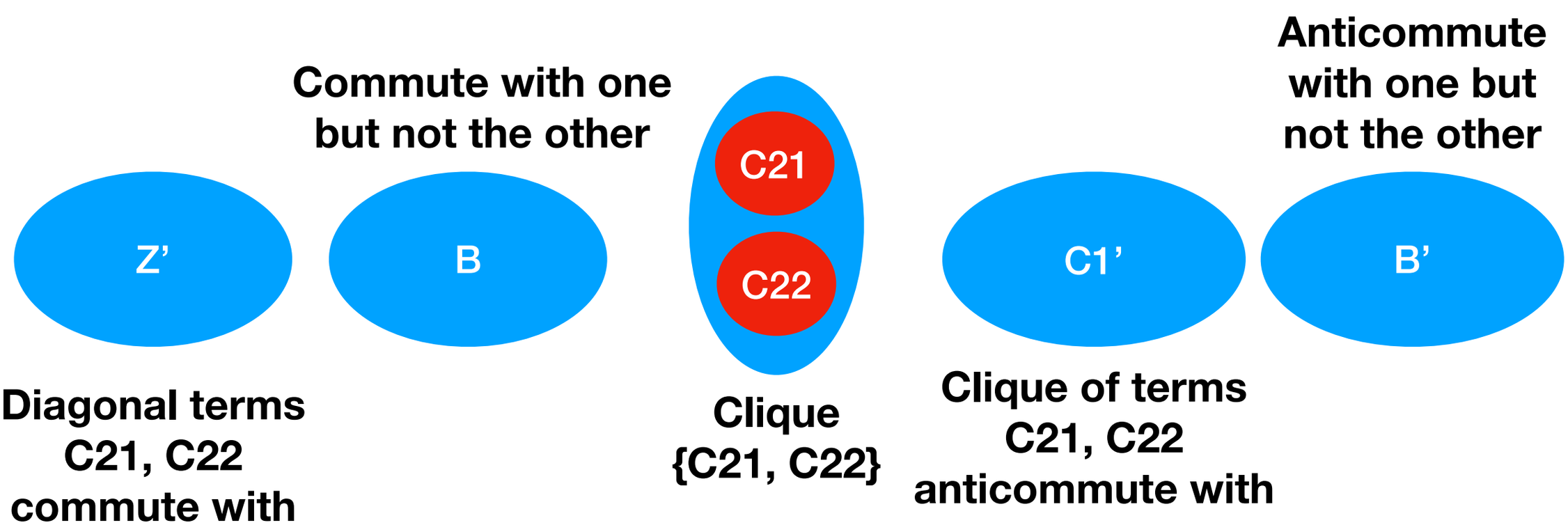
Clique of terms C21 anticommutes with

Now try growing C21. Add another off-diagonal term that commutes with C21. It must have even numbers of X or Y or Z where C21 has distinct even numbers of X or Y or Z, or it may have Pauli operators in places where C21 has identity.

E.g C12 = IXX, C22 = YY, or C22 = YII.

In the first case C22 acts on the same orbitals as C21, and so arises from the same electronic structure term.

In the second case we break the non-contextual structure



B, B’ break the noncontextual structure.

Note, we could fix this by removing diagonal terms, but when HF dominates this gives worse approximation in the examples we have looked at.

What kind of classical quantum chemistry method is NC VQE?

Don’t expect miracles: NC condition is quite strict.

HF is a noncontextual approximation.

Because NC VQE is careful about symmetry in the Hamiltonian, it can outperform HF in settings where multi reference character arises from symmetries alone.

Future work: Different choices of partition into C and NC parts can give an NC Hamiltonian that is NOT HF. Future work!

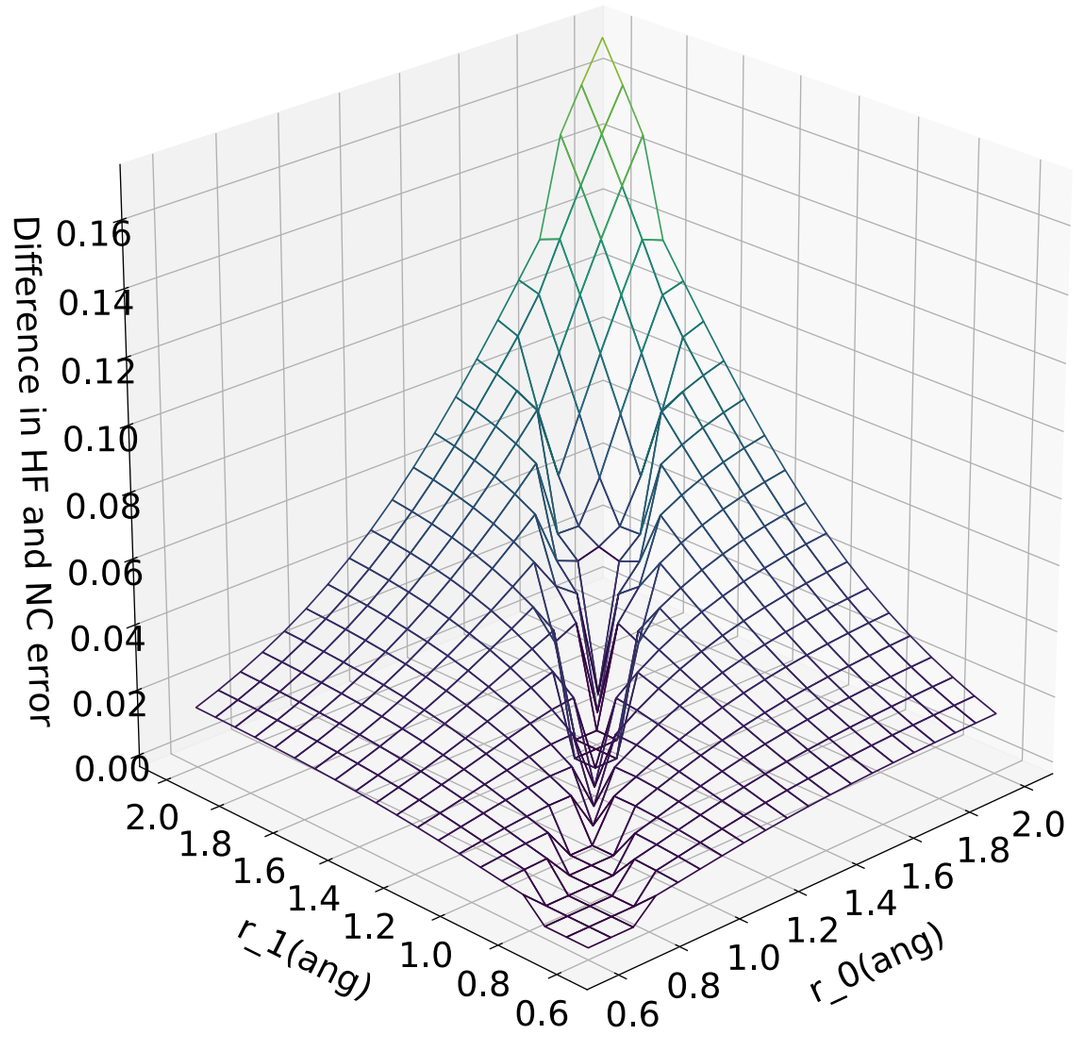


FIG. 3. The difference in error in ground state energy between using the noncontextual approximation and restricted open-shell Hartree Fock, for the H3 potential energy surface. The noncontextual approximation does not suffer from the poor performance of Hartree-Fock at large bond lengths.

To do:

1) Provide good approximate classical methods (and performance bounds) for dividing a Hamiltonian into Contextual and Non-Contextual parts

2) Provide good approximate classical methods (and performance bounds) for solving non-contextual Hamiltonian problems.

3) Apply to LARGE instances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