Contextuality and Variational Quantum Eigensolvers

Raman Choudhary

Outline

1. Variational Quantum Algorithms (VQAs).
2. Contextuality test for Variational Quantum Eigensolvers (VQEs).
3. Classical Simulation of Non-Contextual VQE procedures.
4. Contextual Subspace VQE.

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- Contextuality test for Variational Quantum Eigensolvers (VQEs).
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- Contextual Subspace VQE.

Why Variational Quantum Algorithms??

Traditional practical algorithms like Shor's algorithm, Grover's Algorithm, Quantum Linear System Algorithm have huge resource demands, require error free operations which is incompatible with the current Hardware defining the NISQ era.

Practical Resource Requirements

Factoring a 2048-bit RSA number demands a quantum processor with 10^5 logical qubits and a circuit width of order 10^9.
(Jones et al., 2012- Phys. Rev. X **2**, 031007)

Solving a linear system of equations of size ~ $3 * 10^8$ requires roughly a circuit width of 350 and a depth of order 10^{25} (excluding the oracle calls).
(Artur et al. 2017, Quantum Inf. Process **16,** 60)

	#gates		depth		#qubits
k	T	Clifford	T	overall	
128	$1.19 \cdot 2^{86}$	$1.55 \cdot 2^{86}$	$1.06 \cdot 2^{80}$	$1.16 \cdot 2^{81}$	$2,953$
192	$1.81 \cdot 2^{118}$	$1.17 \cdot 2^{119}$	$1.21 \cdot 2^{112}$	$1.33 \cdot 2^{113}$	$4,449$
256	$1.41 \cdot 2^{151}$	$1.83 \cdot 2^{151}$	$1.44 \cdot 2^{144}$	$1.57 \cdot 2^{145}$	6,681

Table 5. Quantum resource estimates for Grover's algorithm to attack AES-k, where $k \in \{128, 192, 256\}$.

Markus et al., 2015, arXiv:1512.04965v1[quant-ph]

NISQ devices can't afford:

- The huge overload of physical Qubits necessary for QEC to provide useful number of logical qubits.
- High-fidelity operations such that the accumulated error over a significant depth is low enough.
- Error-free readouts.

Current width ~ 50-100 Qubits (no QEC)
Current depth ~100s of Operations

What can be done then?

Best Answer currently is to use Variational Quantum Algorithms.

Variational Quantum Algorithms (VQAs) are hybrid Algorithms which use a Quantum Computer (QC) and a Classical Computer (CC) “repeatedly” to arrive at an approximation to the problem’s solution.

Building Blocks of VQA

- Objective/Cost function- Encode the problem in the form of Hamiltonian Expectation value or some other objective function.
- Parametrised Quantum Circuit (PQC)/Ansatze - intended to map the initial state to a subspace containing the desired (solution) state.
- Classical Optimizer.

$$\langle H \rangle_{\mathcal{U}(\boldsymbol{\theta})} \equiv \langle 0 | \mathcal{U}^{\dagger}(\boldsymbol{\theta}) H \mathcal{U}(\boldsymbol{\theta}) | 0 \rangle$$

$$\min_{\boldsymbol{\theta}} O\left(\boldsymbol{\theta}, \{\langle H \rangle_{\mathcal{U}(\boldsymbol{\theta})}\}\right)$$

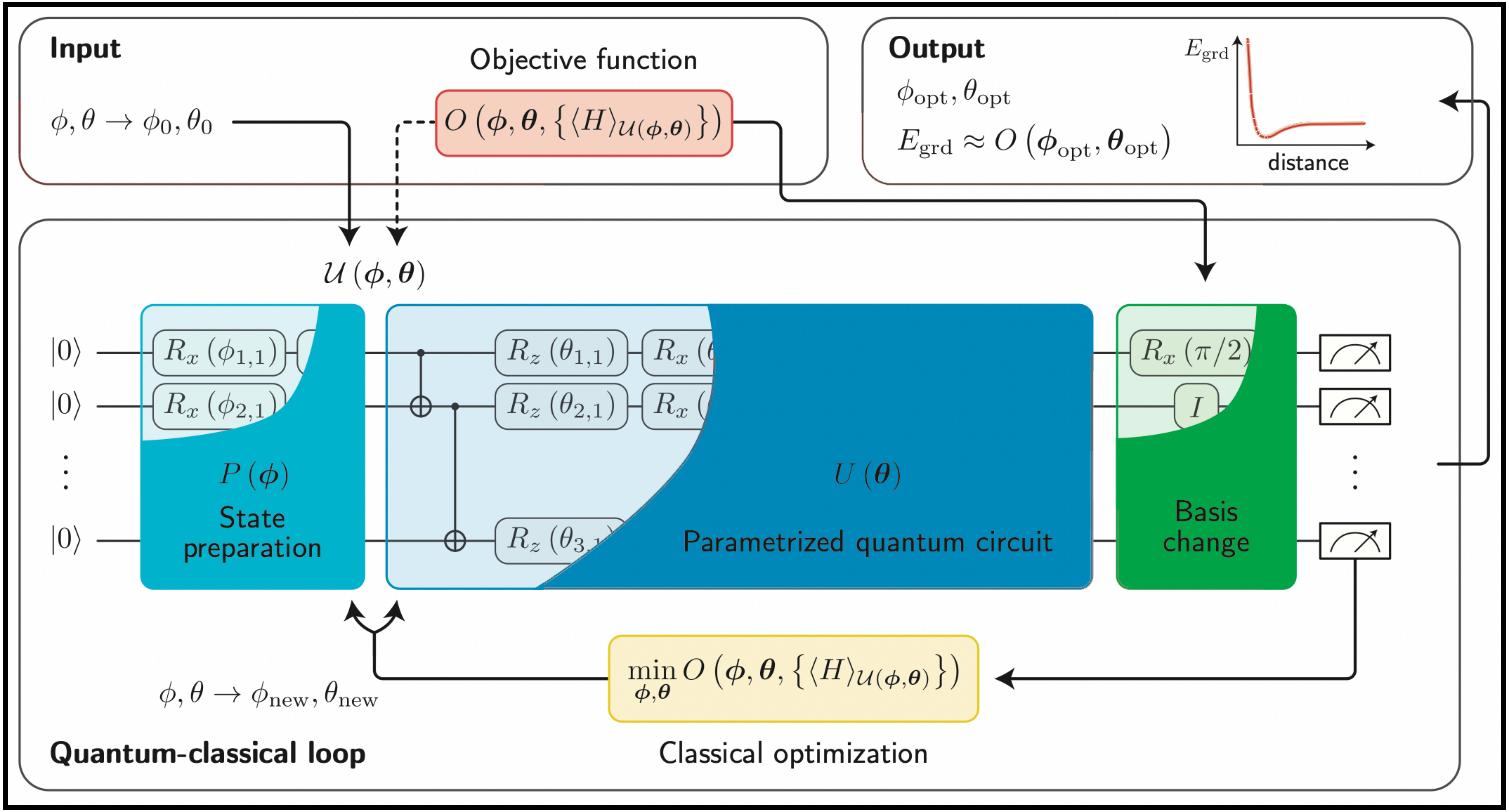

Image taken from: Bharti et al., 2021, arXiv:2101.08448[quant-ph]

Advantages of VQAs

- **Trading off high Coherence time with repetitions** - Since focus is to reach the solution iteratively hence large coherence time isn't needed.

- **Robustness to Noise** - Unless the Noise isn't displacing the final subspace too far from the intended subspace one can just wait till the convergence is achieved.

- **Mapping practically useful algorithms to their VQA versions-** like the Variational Quantum Factoring, Variational Quantum Linear System Solver, etc.

Scope of Work in VQAs

- Ansatze affects Convergence speed and Closeness of final state with the optimal state- Hence **Problem inspired Ansatze** preparation techniques need to be developed.

- **Barren plateau** region escaping techniques during gradient descent classical optimisers.

- **Measurement Reduction techniques.**

- Almost no work on **Energetic advantages** in the literature (upto my best knowledge).

- **Contextuality test of the Ansatze**.

Variational Quantum Eigensolver (VQE)

- Given an n-qubit Hamiltonian H , find its Ground State and Ground State energy. Since n-qubit Paulis form a basis for the n-dimensional Hermitian Operators (with real coefficients):

$$\mathcal{H} = \sum_{i\alpha} h^i_\alpha \sigma^i_\alpha + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta} \sigma^i_\alpha \sigma^j_\beta + \ \dots$$

- Linearity of the Observables:

$$\langle \mathcal{H} \rangle = \sum_{i\alpha} h^i_\alpha \langle \sigma^i_\alpha \rangle + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta} \langle \sigma^i_\alpha \sigma^j_\beta \rangle + \ \dots$$

Peruzzo et al., 2014, Nat. Commun. **5,** 4213

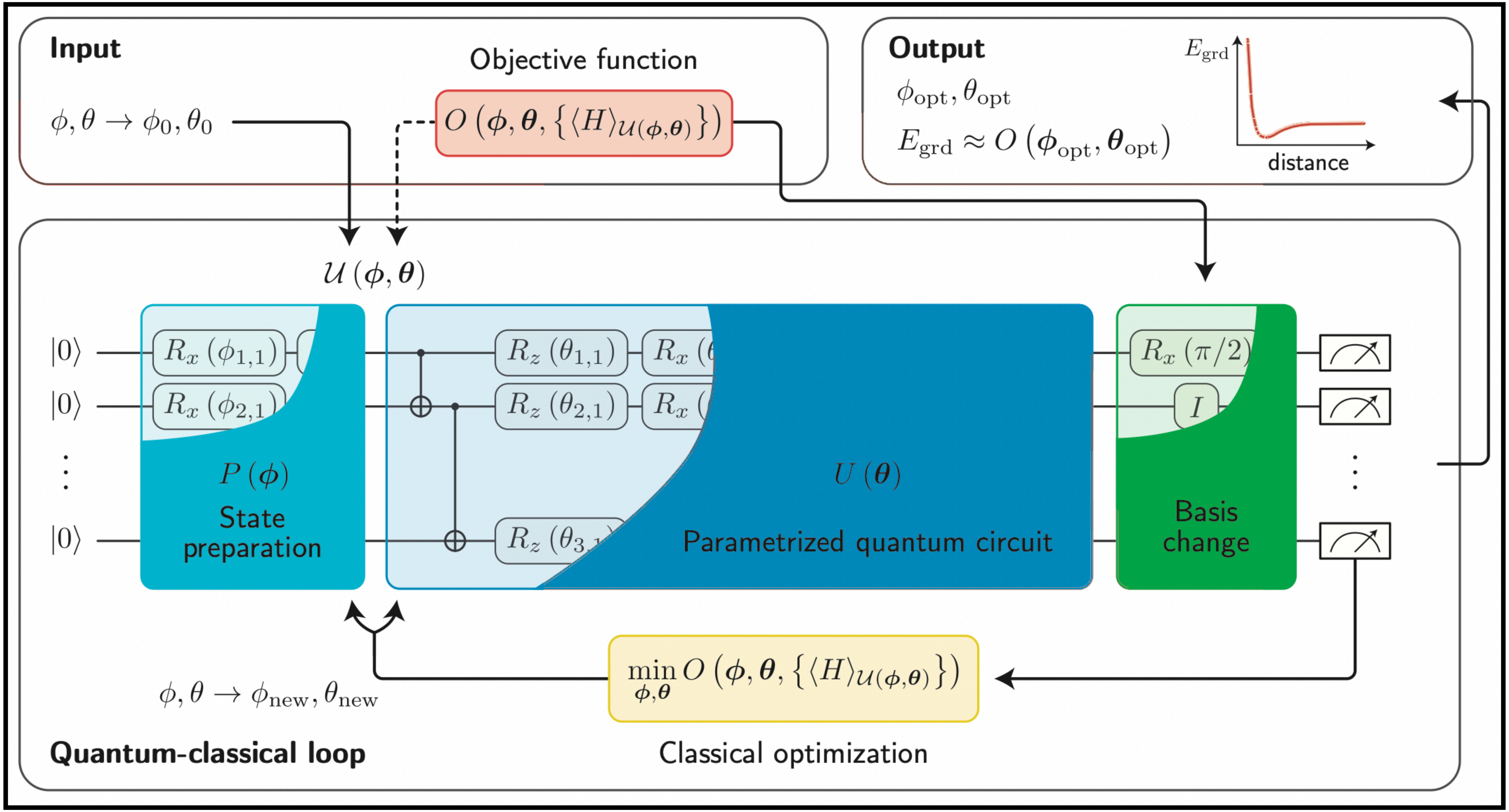

Image taken from: Bharti et al., 2021, arXiv:2101.08448[quant-ph]

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- **Contextuality test for Variational Quantum Eigensolvers (VQEs).**
- Classical Simulation of Non-Contextual VQE procedures.
- Contextual Subspace VQE.

What is Quantum Contextuality?

It is a “special” condition on the Hidden Variable model trying to reproduce the predictions of Quantum Mechanics. The condition is that the value assigned to an observable must depend on what other observables are being measured with it, hence the term “Context” for value assignment.

Approaches to study Contextuality

- **Bell-Kochen-Specker (BKS)** - Given a set of Observables and a set of contexts over this set, assign values* to these Observables and if you arrive at a logical inconsistency/contradiction it means this set exhibits Contextuality.

- **Violating Non-Contextuality Inequalities** - Provided a set of Observables, say X, and a set, say C, of Contexts over X, one then assumes joint Probability distributions over X and derives correlations over Contexts in C which turn out to form a Polytope. Now, if we can find a quantum state such that it predicts a correlation outside this polytope, it means this set exhibits Contextuality.

* in a functionally consistent way

PHYSICAL REVIEW LETTERS **123,** 200501 (2019)

Contextuality Test of the Nonclassicality of Variational Quantum Eigensolvers

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Contextuality is an indicator of nonclassicality, and a resource for various quantum procedures. In this Letter, we use contextuality to evaluate the variational quantum eigensolver (VQE), one of the most promising tools for near-term quantum simulation. We present an efficiently computable test to determine whether or not the objective function for a VQE procedure is contextual. We apply this test to evaluate the contextuality of experimental implementations of VQE, and determine that several, but not all, fail this test of quantumness.

DOI: 10.1103/PhysRevLett.123.200501

Contextuality test of the VQE procedure

- The approach taken is the BKS approach: Given a set of Observables, assign values **<u>in a functionally consistent manner</u>** to these Observables and if you arrive at a logical inconsistency/contradiction it means this set exhibits Contextuality.

- Functional consistency means that if $[\hat{A}, \hat{B}] = 0$ and $\hat{C} = f(\hat{A}, \hat{B})$ then the value assigned to the observable $\hat{C} = f(\hat{A}, \hat{B})$ will be $v(\hat{C}) = f(v(\hat{A}), v(\hat{B}))$.

$$H = \sum_i h_i P_i$$

$$S \equiv \{P_i\}$$

Now construct a Closed Subtheory of $S \equiv \bar{S}$

$\bar{S}$ is the set of all observables whose value can be “inferred” from the values assigned to observables in S.

Inference ??

Inference here means that if

$$[\hat{A}, \hat{B}] = 0 \Longrightarrow \hat{A}\hat{B} \in \bar{S}$$

Closer look at the Sub-theory

$\bar{S}$ contains both Directly and Indirectly inferable observables from S.

$\hat{A}, \hat{B} \in S$ s.t. $[\hat{A}, \hat{B}] = 0$ and $\hat{C}, \hat{D} \in S$ s.t. $[\hat{C}, \hat{D}] = 0$

$\hat{A}\hat{B}$, $\hat{C}\hat{D} \in \bar{S}$ are called Directly Inferable Observables

Now if $[\hat{A}\hat{B}, \hat{C}\hat{D}] = 0$ then $\hat{A}\hat{B}\hat{C}\hat{D} \in \bar{S}$

This $\hat{A}\hat{B}\hat{C}\hat{D}$ is called the indirectly inferred Observable meaning that its value will not be inferred in 1 step after the assignment of values to S.

Explicit Example

$$S = \{I \otimes X, X \otimes I, Z \otimes I, I \otimes Z\}$$

$$\bar{S} = \{I \otimes X, X \otimes I, Z \otimes I, I \otimes Z, Z \otimes X, X \otimes Z, X \otimes X, Z \otimes Z, ZX \otimes XZ, XZ \otimes XZ\}$$

Directly Inferred

Indirectly Inferred

Definition of Contextuality for Hamiltonian

$$H = \sum_i h_i P_i$$

$$S \equiv \{P_i\}$$

Construct $\bar{S}$

Value assignment inconsistency in $\bar{S}$ $\implies$ Contextuality

The authors call this “Strong Contextuality”

Example of this Logical Inconsistency??

$$S = \{I \otimes X, X \otimes I, Z \otimes I, I \otimes Z\}$$

$$\bar{S} = \{I \otimes X, X \otimes I, Z \otimes I, I \otimes Z, Z \otimes X, X \otimes Z, X \otimes X, Z \otimes Z, ZX \otimes XZ, XZ \otimes XZ\}$$

v_1 $\qquad$ v_2 $\qquad$ $v_1 v_2$

$I \otimes X$ $\qquad$ $Z \otimes I$ $\qquad$ $Z \otimes X$

v_3 $\qquad$ v_4 $\qquad$ $v_3 v_4$

$X \otimes I$ $\qquad$ $I \otimes Z$ $\qquad$ $X \otimes Z$

$v_1 v_2 v_3 v_4$

$ZX \otimes XZ$

$v_1 v_3$ $\qquad$ $v_2 v_4$

$X \otimes X$ $\qquad$ $Z \otimes Z$ $\qquad$ $XZ \otimes XZ = -ZX \otimes XZ$

$v_1 v_2 v_3 v_4$

$$v_i \in \{\pm 1\}$$

v_1 | v_2 | $v_1 v_2$
$I \otimes X$ | $Z \otimes I$ | $Z \otimes X$

v_3 | v_4 | $v_3 v_4$
$X \otimes I$ | $I \otimes Z$ | $X \otimes Z$

$v_1 v_2 v_3 v_4$
$ZX \otimes XZ$

$v_1 v_3$ | $v_2 v_4$
$X \otimes X$ | $Z \otimes Z$ | $XZ \otimes XZ = -ZX \otimes XZ$

$v_1 v_2 v_3 v_4$

Observables $\hat{A}$ and -$\hat{A}$ get assigned the same value contradicting the QM prediction that they can only be Anti-Correlated where $\hat{A}$ is $ZX \otimes XZ = Y \otimes Y$

Hence the set S exhibits Contextuality (the famous Peres-Mermin Square)

Generalizing in terms of Determining tree and Determining set

$$H = \sum_i h_i P_i$$

$$S \equiv \{P_i\}$$

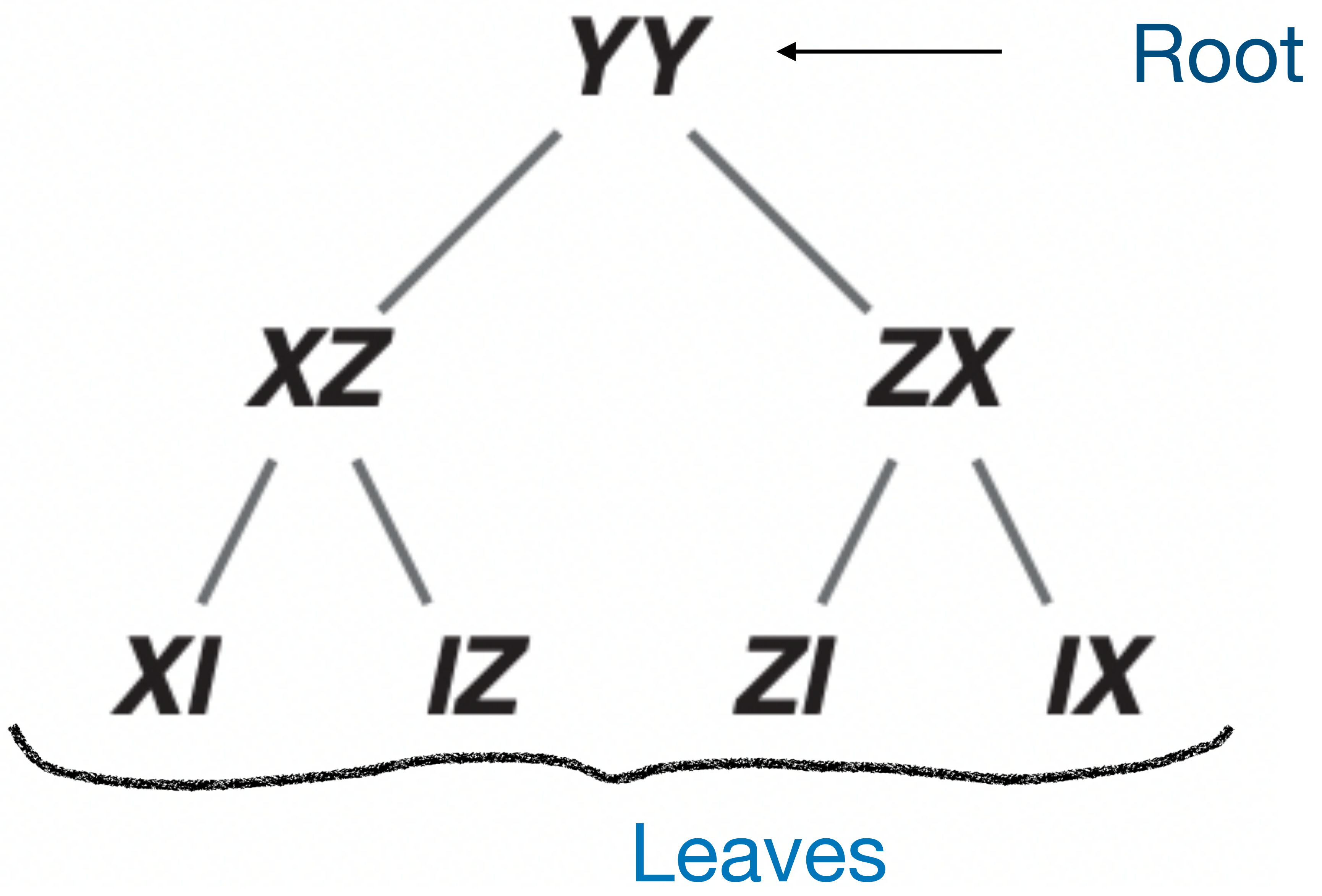
A determining tree τ for a Pauli measurement $A \in \bar{S}$ over a set of Pauli measurements S is a tree whose nodes are Pauli Operators and whose leaves are operators in S such that:

(1) the root of the tree is A

(2) all children of any parent pairwise commute

Any operator in $\bar{S}$ can be represented with a determining tree with leaves in S

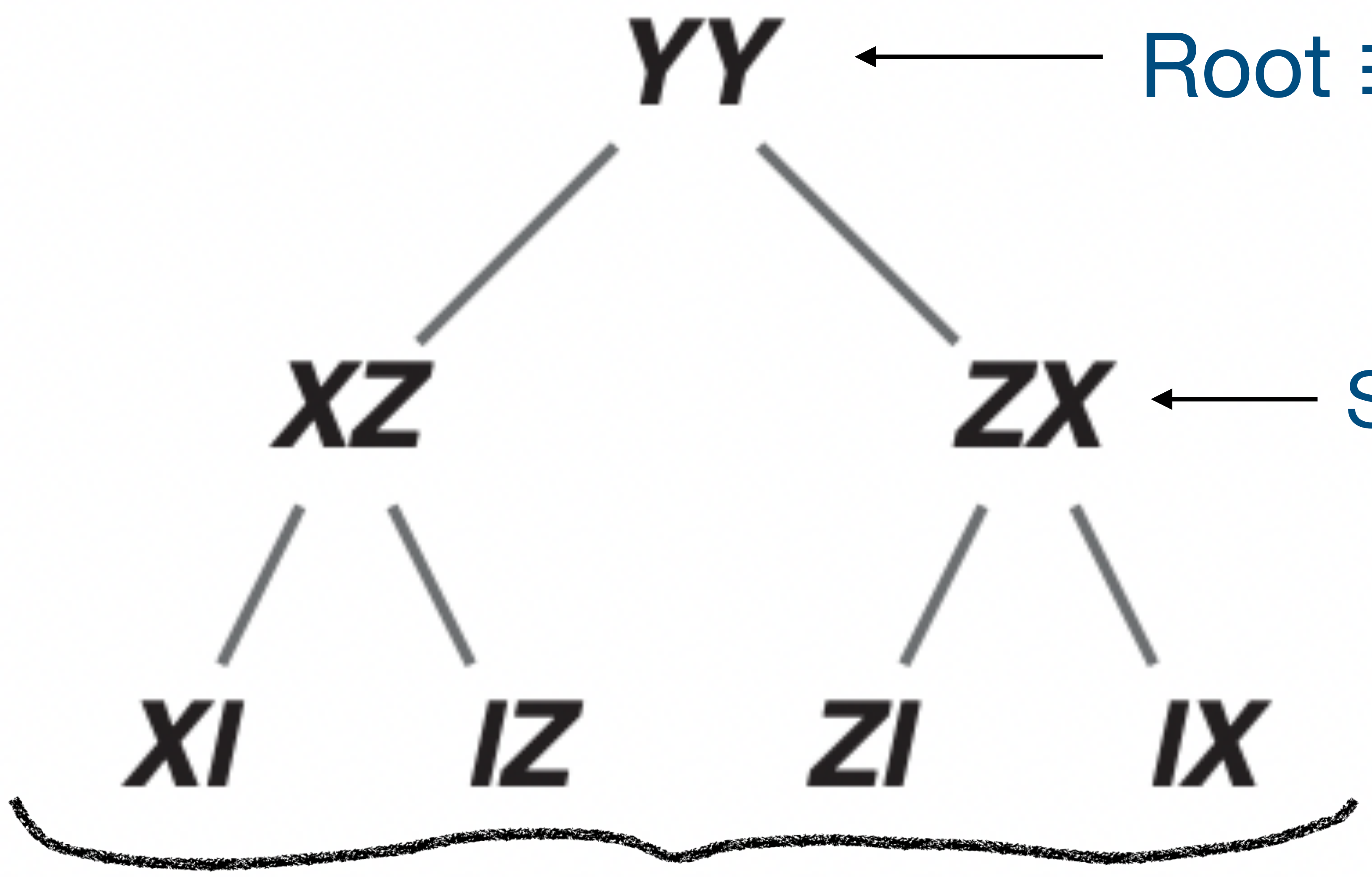
τ for YY in $\bar{S}$



$$S = \{IX, XI, ZI, IZ\}$$

$$\bar{S} = \{IX, XI, ZI, IZ, ZX, XZ, XX, ZZ, YY, -YY\}$$

τ for YY in $\bar{S}$



Root $\equiv$ Node at the top of the tree

Simple Node NOT called Leaf or Root

Leaves $\equiv$ Nodes in the tree which are operators in S

$$YY = (XZ)(ZX) = (XI)(IZ)(ZI)(IX)$$

Eventually, a Root is a product of Leaves

Since we are assigning only ± 1 to the leaves, this means that only those leaves will contribute to the assignment of the root which occur odd number of times.

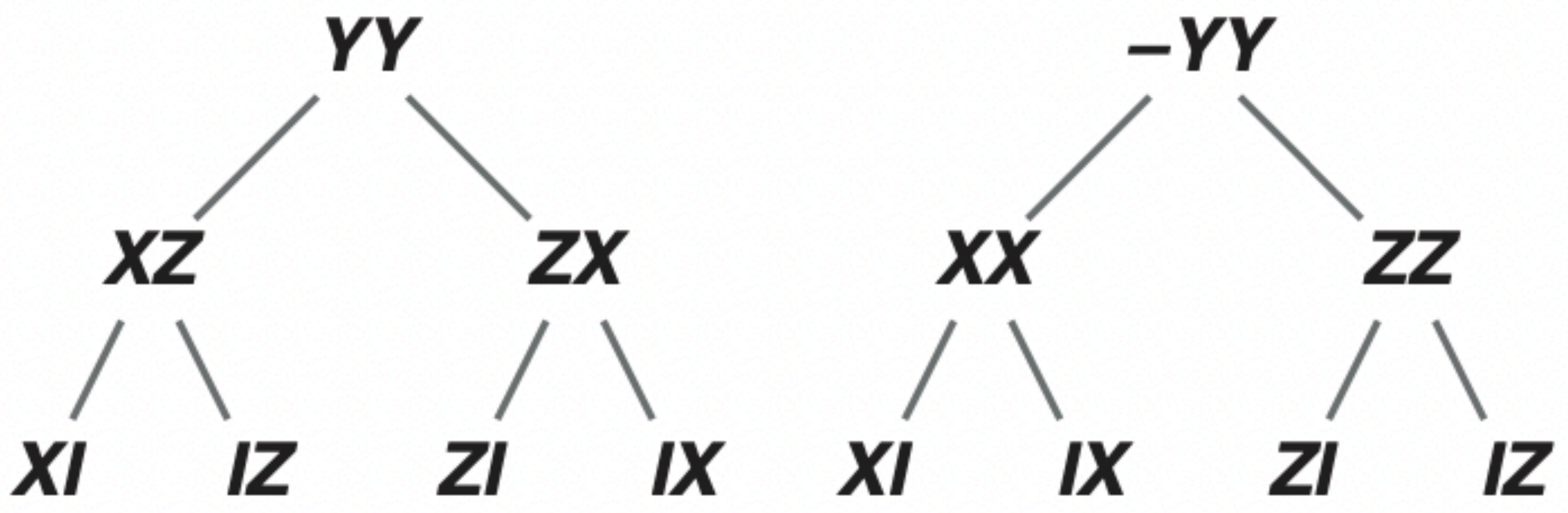
For a determining tree τ let D be the set of leaves with odd multiplicities then D will be called a Determining set for τ.

Definition of Contextuality

$$H = \sum_i h_i P_i$$

$$S \equiv \{P_i\}$$

A set S of Pauli Observables is called Contextual if for some Pauli $A \in \bar{S}$ there exists a determining tree τ over S and a determining tree τ' for -A over S such that they have identical Determining Sets.



Determining trees for $\pm YY$ over $\{XI, IX, ZI, IZ\}$.

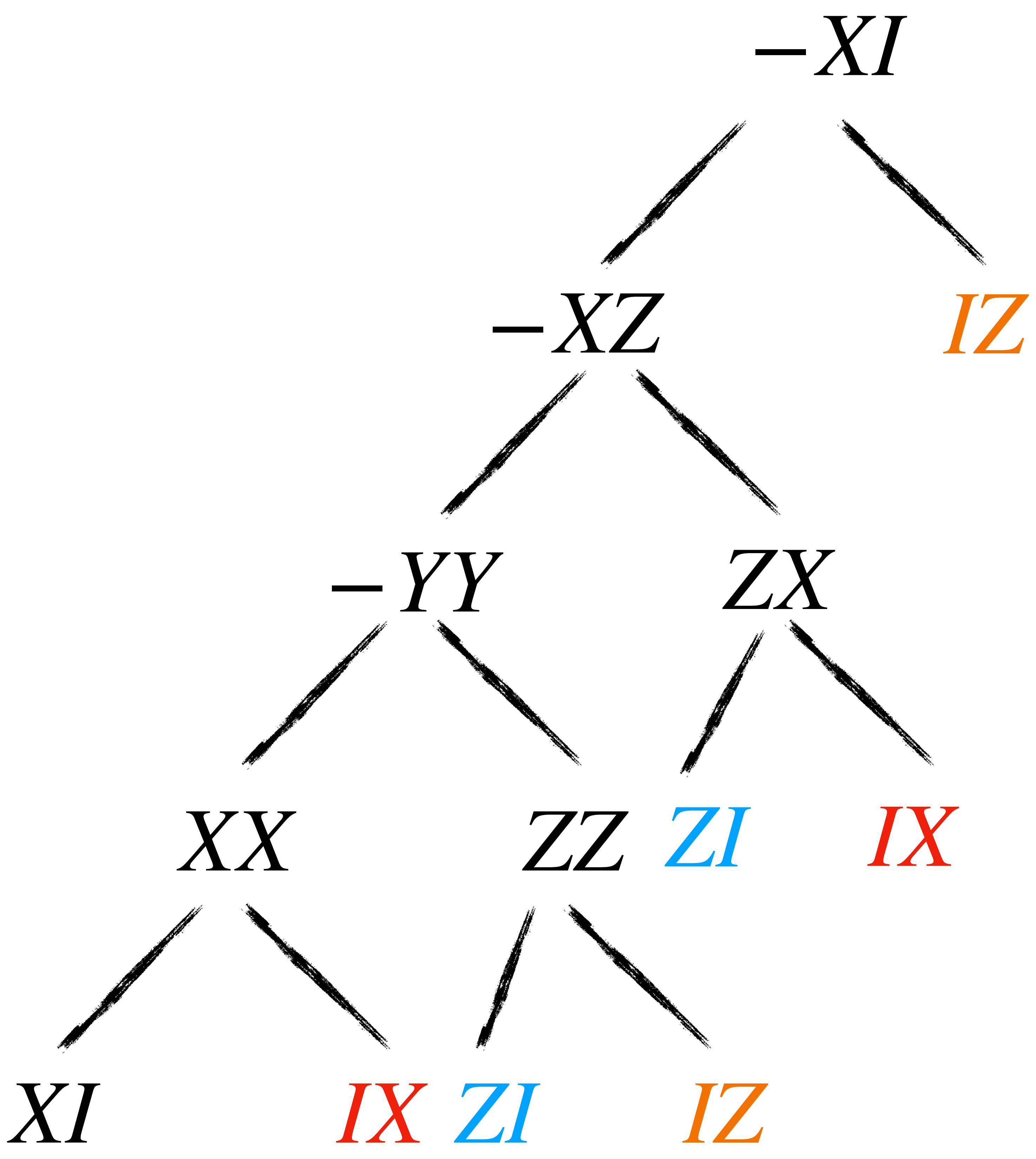
$$YY = (XZ)(ZX) = (XI)(IZ)(ZI)(IX)$$
$$-YY = (XX)(ZZ) = (XI)(IX)(ZI)(IZ)$$

Necessary and Sufficient conditions for Contextuality

Condition 1

A set S of Pauli operators is Contextual iff for some $\hat{B} \in S$ there exists a determining tree for -$\hat{B}$ over S, whose determining set is $\{B\}$.

$$S = \{IX, XI, ZI, IZ\}$$



Among all the leaves only XI has odd multiplicity, hence determining set of $-XI$ is $\{XI\}$.

$$-XI = (XI)(IX)(ZI)(IZ)(ZI)(IX)(IZ)$$

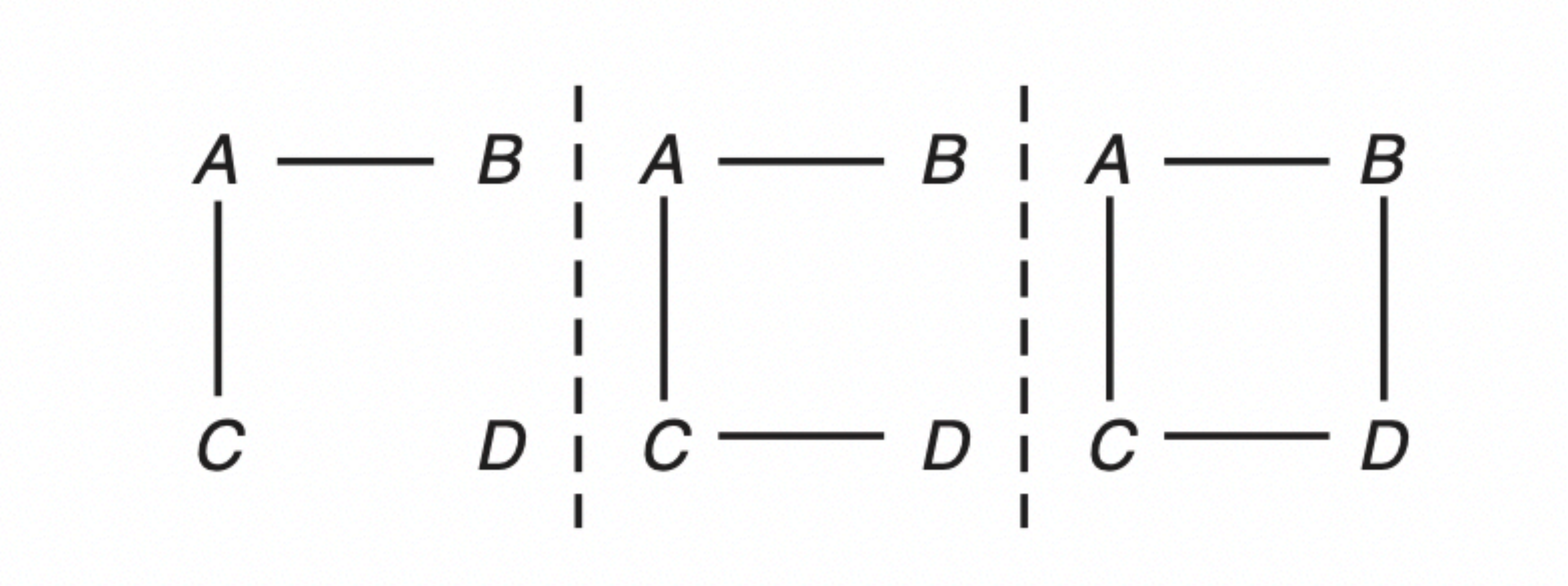
Condition 2

A set S of Pauli Observables is Contextual iff there exists a determining tree of $-I$ over S such that the determining set is empty.

Effectively it means that $-I$ gets an assignment of +1 contradicting QM.

Condition 3

A set S of Pauli Operators is Contextual iff it contains a subset consisting of four operators whose compatibility graph has one of the following forms:



Rough Sketch of the proof of Condition 3

"If" part :

From such subgraphs one can construct a determining tree of $-I$ over S with an empty determining set, hence by Condition 2, S will be Contextual.

"Only if" part :

(i) removal of Casimirs* from S, call the remaining set T.

(ii) a proof that over T transitivity of Commutation can't hold.

* Universally Commuting elements

Necessary and Sufficient Condition for noncontextuality

Given a set S of Pauli Observables, let $T \subseteq S$ be the set obtained by removing the Casimirs from S.

S is noncontextual iff transitivity of Commutation holds on T.

Since Commutation is by definition:

(i) Reflexive - $[\hat{A}, \hat{A}] = 0$
(ii) Symmetric - if $[\hat{A}, \hat{B}] = 0$ then $[\hat{B}, \hat{A}] = 0$.

So presence of transitivity over T makes Commutation an equivalence relation on T.

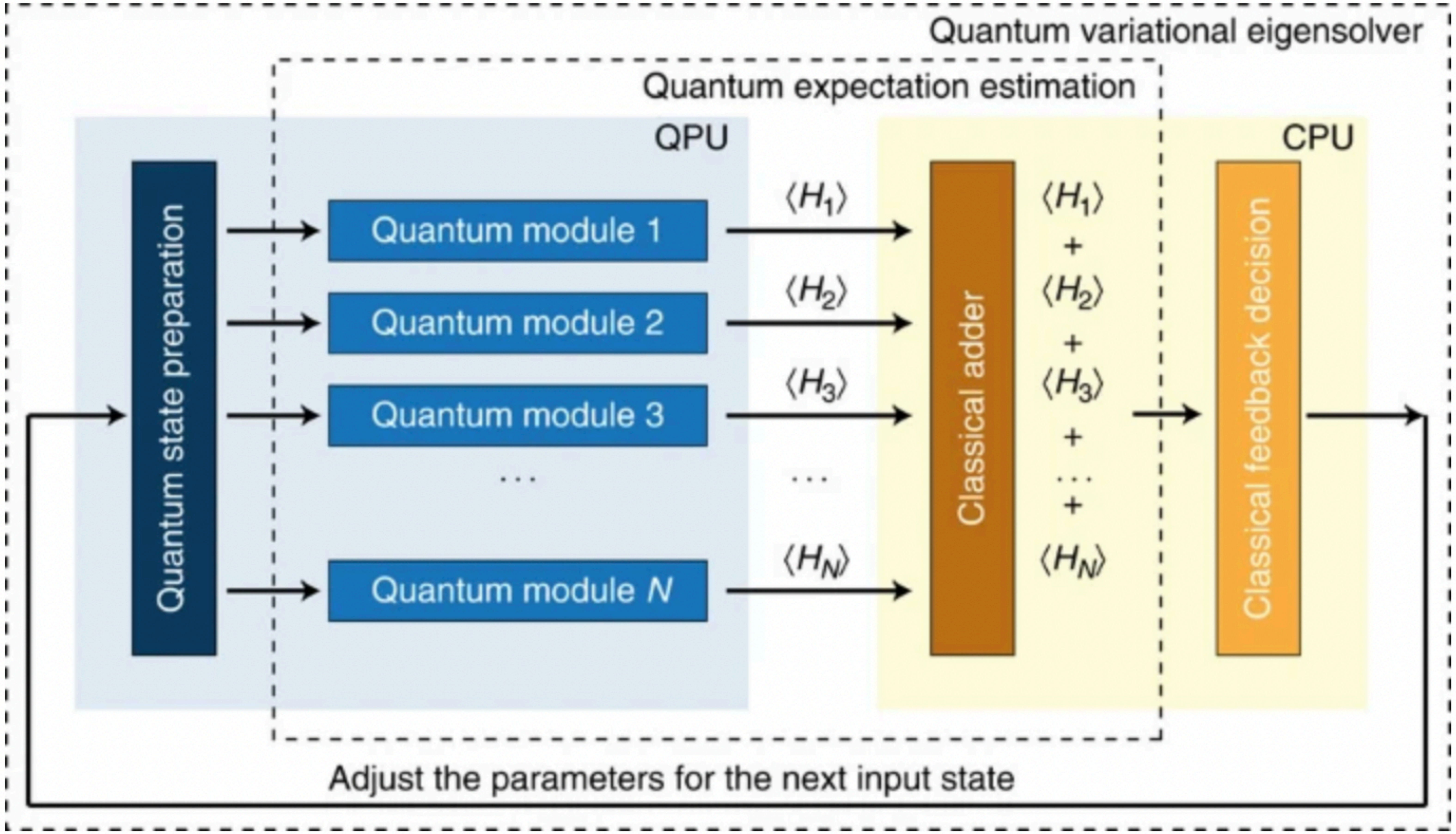
TABLE I. Evaluation of contextuality in VQE experiments. CD_0 is the minimum number of terms we must remove from the Hamiltonian to reach a noncontextual set, as a fraction of the total number of terms ($|\mathcal{S}|$). In [22], $|\mathcal{S}|$ varies.

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	~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	~0.74	164
Kandala *et al.* [17,21]	LiH	Yes	~0.77	99

Kirby et al., 2019, Phys. Rev. Lett. **123**, 200501

Remember that all this while Contextuality of S means that one can observe a logical contradiction in value assignment over $\bar{S}$.

although there might be NO contradiction within the elements of S only



$$\langle \mathcal{H} \rangle = \sum_{i\alpha} h^i_\alpha \langle \sigma^i_\alpha \rangle + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta} \langle \sigma^i_\alpha \sigma^j_\beta \rangle + \ \ldots$$

But in a VQE experiment we aren't measuring any observables outside S!!!

Contextuality bounds the efficiency of classical simulation of quantum processes

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Contextuality has been conjectured to be a super-classical resource for quantum computation, analogous to the role of non-locality as a super-classical resource for communication. We show that the presence of contextuality places a lower bound on the amount of classical memory required to simulate any quantum sub-theory, thereby establishing a quantitative connection between contextuality and classical simulability. We apply our result to the qubit stabilizer sub-theory, where the presence of state-independent contextuality has been an obstacle in establishing contextuality as a quantum computational resource. We find that the presence of contextuality in this sub-theory demands that the minimum number of classical bits of memory required to simulate a multi-qubit system must scale quadratically in the number of qubits; notably, this is the same scaling as the Gottesman-Knill algorithm. We contrast this result with the (non-contextual) qudit case, where linear scaling is possible.

Give a quantitative link between Classical Simulation and Contextuality, hence a motivation to investigate if any Quantum Advantage in VQEs is associated with Contextuality.

arXiv:1802.07744[quant-ph]

NC-Inequality approach sticks to the given set

Provided a set of Observables, say S, and a set, say $\mathscr{C}$, of Contexts over S, one then assumes joint Probability distributions over S and derives correlations over Contexts in $\mathscr{C}$ which turn out to form a Polytope.

Now, if we can find a quantum state such that it predicts a correlation outside this polytope, it means this set exhibits Contextuality.

Let us call it “Weak Contextuality”

PHYSICAL REVIEW A **99**, 020103(R) (2019)

Rapid Communications

Necessary and sufficient condition for contextuality from incompatibility

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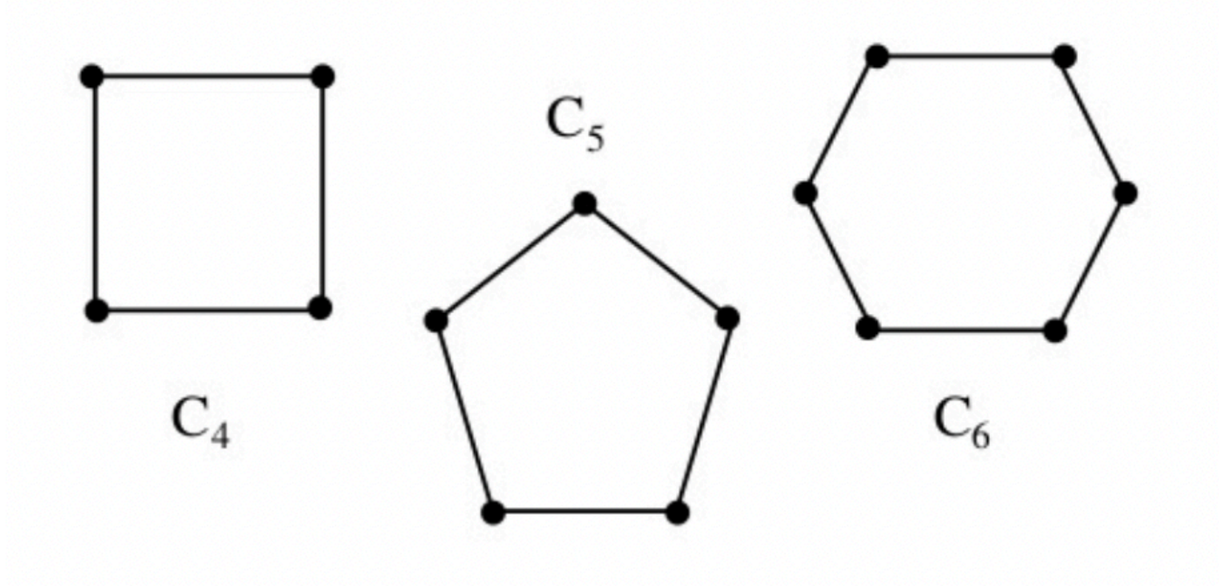
Measurement incompatibility is the most basic resource that distinguishes quantum from classical physics. Contextuality is the critical resource behind the power of some models of quantum computation and is also a necessary ingredient for many applications in quantum information. A fundamental problem is thus identifying when incompatibility produces contextuality. Here, we show that, given a structure of incompatibility characterized by a graph in which nonadjacent vertices represent incompatible ideal measurements, the necessary and sufficient condition for the existence of a quantum realization producing contextuality is that this graph contains induced cycles of size larger than three.

DOI: 10.1103/PhysRevA.99.020103

Vorobyev's Theorem tells that Non-chordality is necessary for Contextuality - here they prove that it is also sufficient.

Non-Chordality of a Compatibility graph $\Longleftrightarrow$ Quantum Contextuality

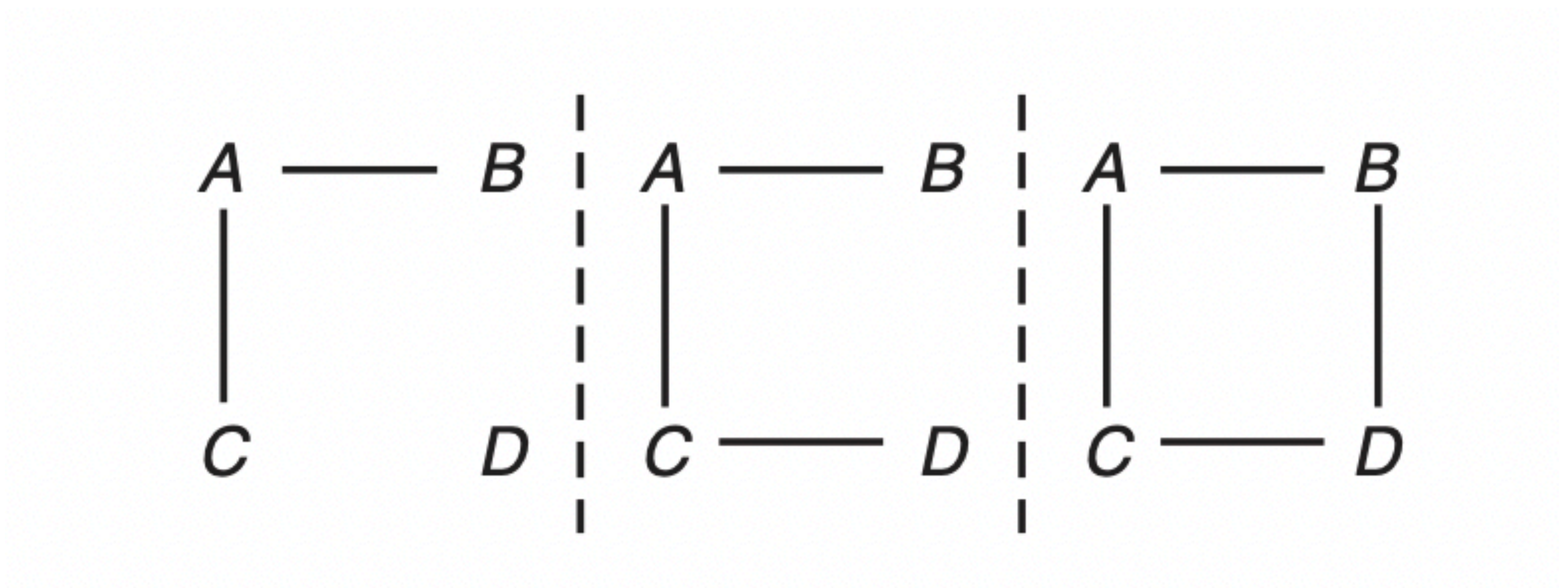
Non-Chordality means that the graph has at least one cycle of size ≥ 4 with no chord (edge between non-adjacent vertices)



Notice here that Contextuality for S means that experimental statistics of S only can't be reproduced by any underlying hidden variable model.
(No reference of anything outside S).

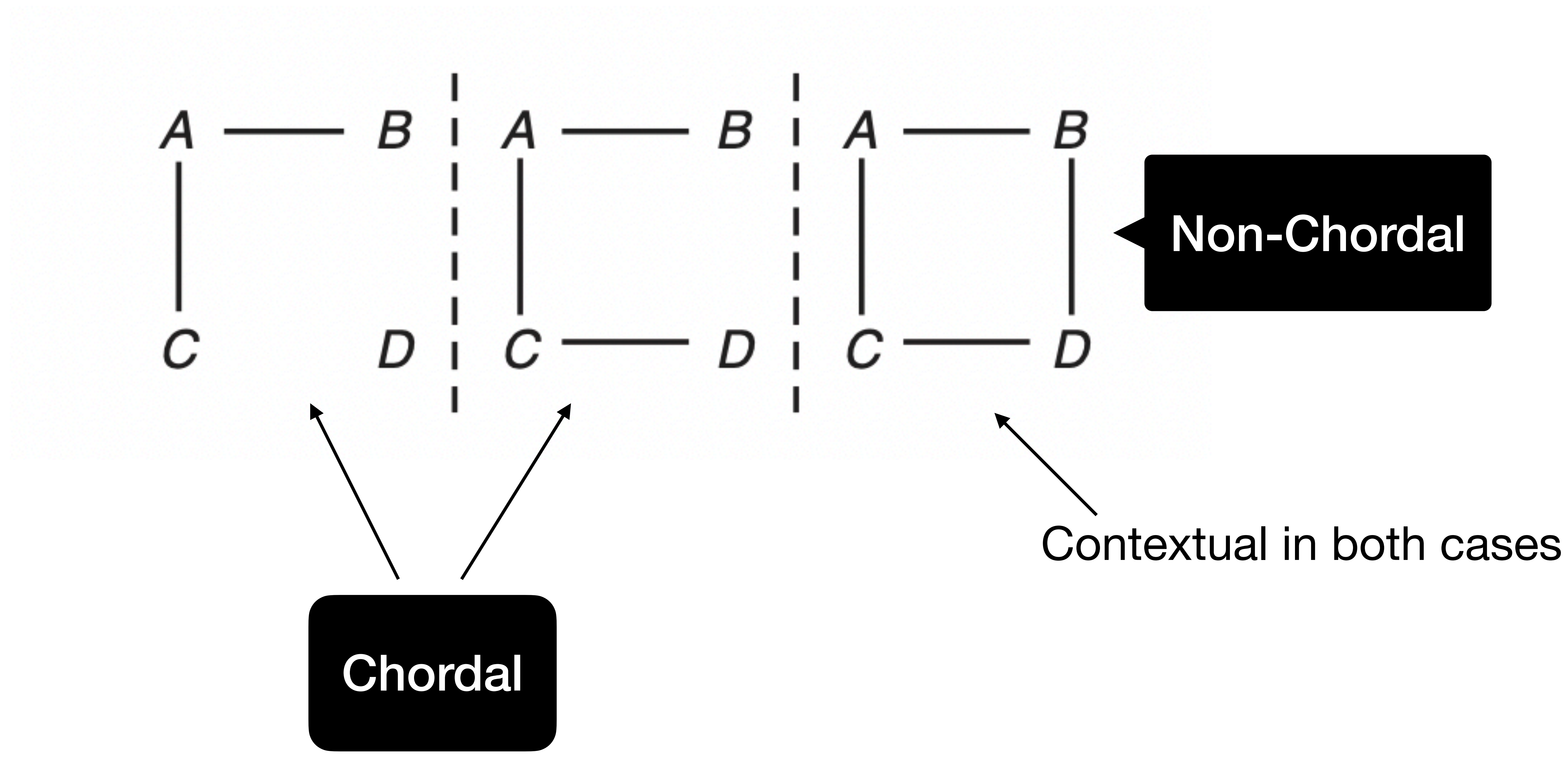
Let us call it "Weak Contextuality"

Comparing the two scenarios



Presence of these graphs means that this set of 4 observables can be extended to a bigger set exhibiting Value-assignment inconsistency.

Comparing the two scenarios



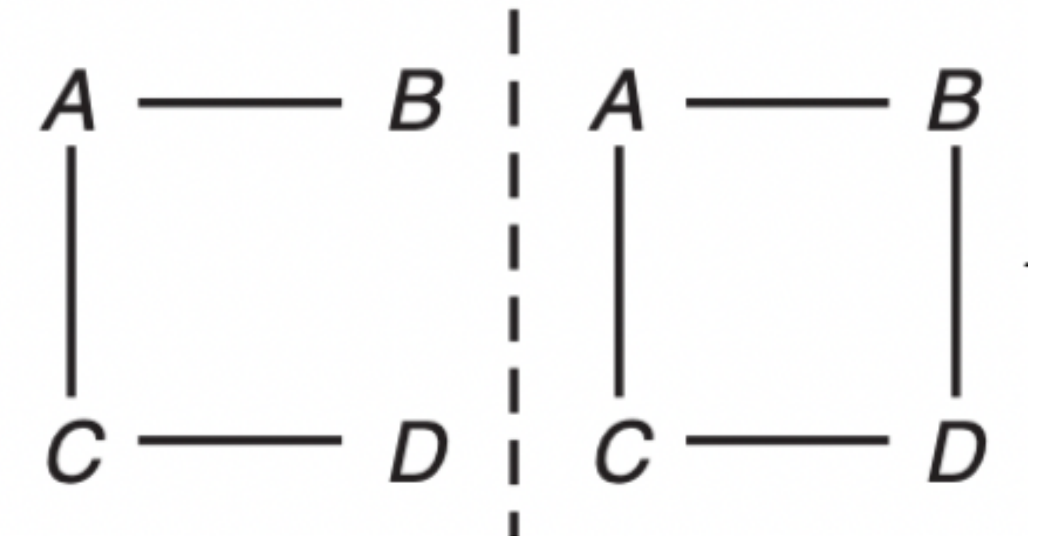
The first two graphs are noncontextual according to the Non-Chordality condition suggesting that a HV model exists if we don't allow any external inclusion of Observables.

Strong Contextuality for $S \not\Rightarrow$ Weak Contextuality for S

Weak Contextuality for $S \Longrightarrow$ Strong Contextuality for S

$\Updownarrow$

Non-Chordality $\Longrightarrow$



As subgraphs

Hence for a set S of Pauli Observables one can always go from SD contextuality to SID Contextuality by expanding the set S to $\bar{S}$.

Open Questions

How Contextuality links with Classical Simulation of non-closed Quantum Subtheories??

What about Strong Contextuality of Non-Pauli sets??

Outline

- Variational Quantum Algorithms (VQAs).
- Contextuality test for Variational Quantum Eigensolvers (VQEs).
- **Classical Simulation of Non-Contextual VQE procedures.**
- Contextual Subspace VQE.

PHYSICAL REVIEW A **102**, 032418 (2020)

Classical simulation of noncontextual Pauli Hamiltonians

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(Received 20 February 2020; accepted 19 August 2020; published 24 September 2020)

Noncontextual Pauli Hamiltonians decompose into sets of Pauli terms to which joint values may be assigned without contradiction. We construct a quasiquantized model for noncontextual Pauli Hamiltonians. Using this model, we give an algorithm to classically simulate the noncontextual variational quantum eigensolver. We also use the model to show that the noncontextual Hamiltonian problem is NP-complete. Finally, we explore the applicability of our quasiquantized model as an approximate simulation tool for contextual Hamiltonians. These results support the notion of noncontextuality as classicality in near-term quantum algorithms.

DOI: 10.1103/PhysRevA.102.032418

Non-Contextual Hamiltonian

$$H = \sum_i h_i P_i$$

$$S \equiv \{P_i\}$$

Given a set S of Pauli Observables, let $T \subseteq S$ be the set obtained by removing
Casimirs from S. Then:

S is noncontextual iff Commutation holds Transitivity over T.

In terms of Compatibility graph of T it means that it is a **Union of disjoint Cliques**.

$$S = T \cup Z$$

where $T = \bigcup_i C_i$ with $C_i = \{C_{i1}, C_{i2}, \dots, C_{i|C_i|}\}$ and $Z = S \backslash T$.

$$S = T \cup Z$$

where $T = \bigcup_i C_i$ with $C_i = \{C_{i1}, C_{i2}, \ldots, C_{i|C_i|}\}$ and $Z = S \backslash T$.

$$H = \sum_{i=1}^{N} \left(\sum_{j=1}^{|C_i|} h_{ij} C_{ij} \right) + \sum_{B \in \mathcal{Z}} h_B B$$

Steps to Construct a Classical Simulation of VQE

Since S is noncontextual therefore joint value assignments on S exist but not every joint assignment would be consistent (since some elements might be products of commuting elements). Then:

1. Obtain an independent set R of Pauli operators from S. From R anything from S to its closed subtheory $\bar{S}$ can be inferred, hence $\bar{R} = \bar{S}$.

2. Obtain Probability Distributions over assignments to R and Parametrise them in such a way that they correspond to Eigenstates of H.

3. Minimise $< H >$ over this parametrised Probability Distribution and obtain the ground state energy & from the optimal parameters one can then construct the Quantum State.

More details* describing each of these steps

* Rough picture

Step 1: Obtaining the independent set R

$$S = T \cup Z$$

where $T = \bigcup_i C_i$ with $C_i = \{C_{i1}, C_{i2}, \ldots, C_{i|C_i|}\}$ and $Z = S \backslash T$.

Construct a set, G', of some Casimirs Inferable from S

$$G' \equiv \mathcal{Z} \cup \left(\bigcup_{i=1}^{N} \{A_{ij} \mid j = 2, 3, \ldots, |C_i|\} \right)$$

$$A_{ij} \equiv C_{ij} C_{i1}$$

here G' will, in general, be a dependent set, so need to obtain an independent set G from G'

$$G' \equiv \mathcal{Z} \cup \left(\bigcup_{i=1}^{N} \{A_{ij} \mid j = 2, 3, \ldots, |C_i|\} \right)$$

$$A_{ij} \equiv C_{ij} C_{i1}$$

here G' will, in general, be a dependent set, so need to obtain an independent set G from it

This can be done by a technique called Multiplicative variant of Gaussian Elimination*

$$\mathcal{R} \equiv \{C_{i1} \mid i = 1, 2, \ldots, N\} \cup G$$

$$S = T \cup Z$$

where $T = \bigcup_i C_i$ with $C_i = \{C_{i1}, C_{i2}, \ldots, C_{i|C_i|}\}$ and $Z = S \backslash T$.

Since G generates G', therefore it generates Z and each element A_{ij}, also each element of T is of the form C_{ij} which can be obtainable my multiplying A_{ij} with C_{i1} from R.

Thus proving that each observable in set S can be obtained as product of commuting elements in R, hence values assigned to R lead to value assignments in S.

* Only applies to Completely Commuting set

Step 2 : Obtain Probability Distributions over assignments to R + Parametrisation

$$\mathcal{R} \equiv \{C_{i1} \mid i = 1, 2, \ldots, N\} \cup G$$

$$v_i \in \{\pm 1\}^{|R|}$$

These Value assignments will be called the Ontic states

Probability distributions (PDs) over the ontic states will define the Epistemic states

$$P(c_1, c_2, \ldots, c_N, g_1, g_2, \ldots)$$

A parametrisation that reproduces the expectation value for eigenstates of Hamiltonian is sufficient to simulate VQE.

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

Step 3 : Minimizing $< H >$ over the PDs

$$H = \sum_{i=1}^{N} \left(\sum_{j=1}^{|C_i|} h_{ij} C_{ij} \right) + \sum_{B \in \mathcal{Z}} h_B B$$

$$A_{ij} \equiv C_{ij} C_{i1}$$

$$H = \sum_{i=1}^{N} \left(\sum_{j=1}^{|C_i|} h_{ij} A_{ij} \right) C_{i1} + \sum_{B \in \mathcal{Z}} h_B B$$

Each A_{ij} and B are product of operators from G and hence belong to $\bar{G}$

$$H = \sum_{B \in \overline{G}} \left(h_B B + \sum_{i=1}^{N} h_{B,i} B C_{i1} \right)$$

where $B = \prod_{j \in \mathcal{J}_B} G_j$

$$H = \sum_{B \in \overline{G}} \left(h_B B + \sum_{i=1}^{N} h_{B,i} B C_{i1} \right)$$

$$B = \prod_{j \in \mathcal{J}_B} G_j$$

$$\langle B \rangle_{(\vec{q},\vec{r})} = \left\langle \prod_{j \in \mathcal{J}_B} G_j \right\rangle = \prod_{j \in \mathcal{J}_B} q_j,$$

$$\langle C_{i1} B \rangle_{(\vec{q},\vec{r})} = r_i \prod_{j \in \mathcal{J}_B} q_j$$

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

This is in general a non-convex function whose global minima gives the ground state energy.

In general finding the ground state energy of a Hamiltonian is QMA-hard but the noncontextual Hamiltonian problem is only NP-complete.

At worst Classically Hard

Outline

- Variational Quantum Algorithms (VQAs).
- Contextuality test for Variational Quantum Eigensolvers (VQEs).
- Classical Simulation of Non-Contextual VQE procedures.
- **Contextual Subspace VQE.**

Contextual Subspace Variational Quantum Eigensolver

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We describe *contextual subspace variational quantum eigensolver* (CS-VQE), a hybrid quantum-classical algorithm for approximating the ground state energy of a Hamiltonian. The approximation to the ground state energy is obtained as the sum of two contributions. The first contribution arises from a noncontextual approximation to the Hamiltonian, and is computed classically. The second contribution is obtained by using the variational quantum eigensolver (VQE) technique to compute a contextual correction on a quantum processor. In general the VQE computation of the contextual correction uses fewer qubits and measurements than the VQE computation of the original problem. Varying the number of qubits used for the contextual correction adjusts the quality of the approximation. We simulate CS-VQE on tapered Hamiltonians for small molecules, and find that the number of qubits required to reach chemical accuracy can be reduced by more than a factor of two. The number of terms required to compute the contextual correction can be reduced by more than a factor of ten, without the use of other measurement reduction schemes. This indicates that CS-VQE is a promising approach for eigenvalue computations on noisy intermediate-scale quantum (NISQ) devices.

Kirby et al., 2020, arXiv:2011.10027 **[quant-ph]**

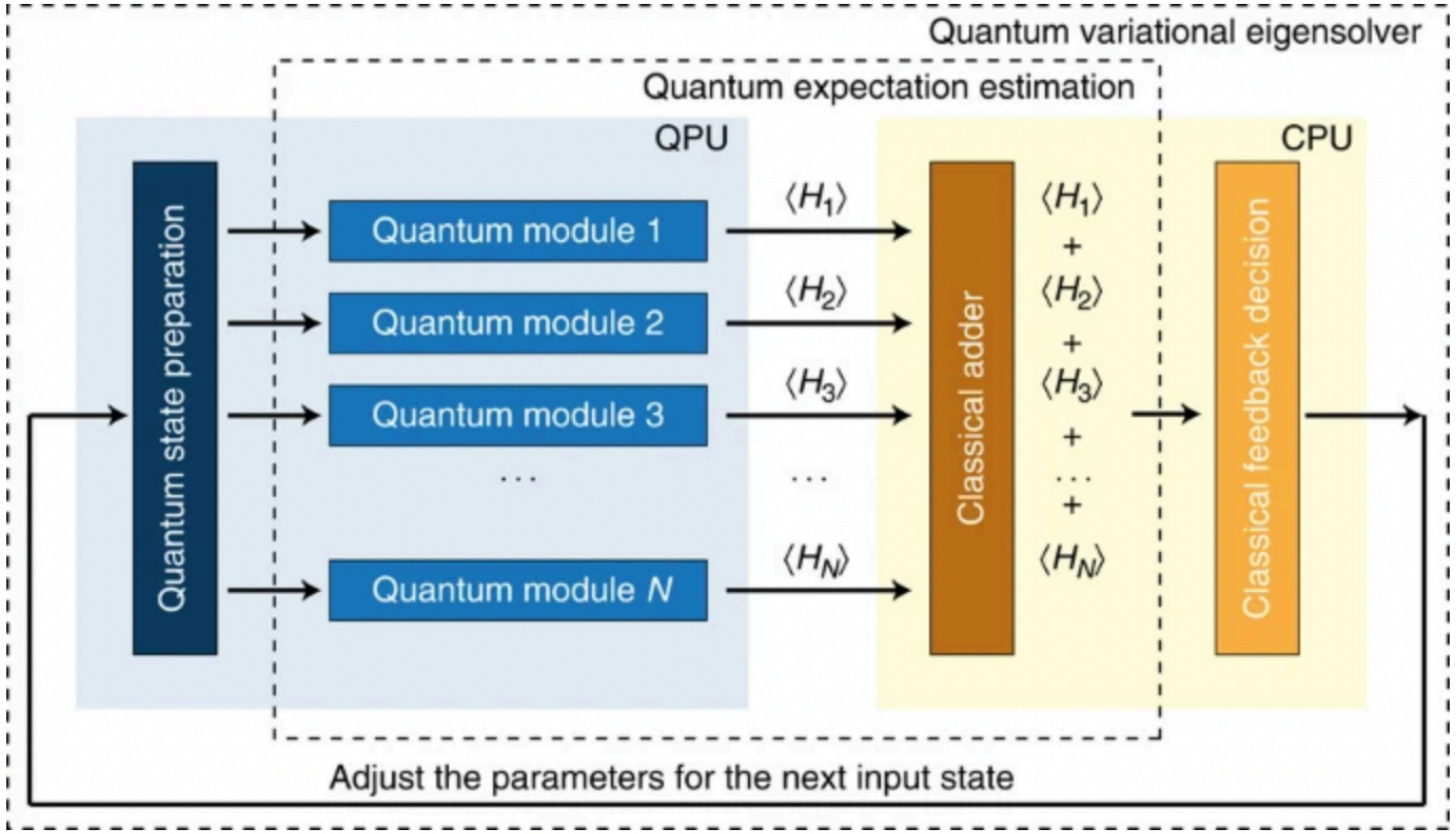
Contextual Subspace VQE

A Quantum-Classical hybrid algorithm which computes approximations to ground state energy of an n-qubit Hamiltonian as a sum of two contributions:
(i) Non-Contextual Contribution (Classical).
(ii) Quantum Correction over (i) using VQE on less than n Qubits.

Note: No Intention to prepare the ground state

Motivation for Contextual subspace VQE

In a usual VQE scenario, at the end of each iteration over the Quantum Circuit, large number of measurements are needed to be done to compute expectation value of the Complete Hamiltonian.



$$\langle \mathcal{H} \rangle = \sum_{i\alpha} h^i_\alpha \langle \sigma^i_\alpha \rangle + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta} \langle \sigma^i_\alpha \sigma^j_\beta \rangle + \ \dots$$

So is it possible to delegate as much Computation as possible to the Classical Computer and still achieve good approximations to ground state energy??

Maybe Contextual Subspace VQE could help since it reduces overload from the noisy QC.

Given a general n-qubit hamiltonian H

$$H = \sum_i h_i P_i$$

$$S \equiv \{P_i\}$$

Divide S into a Non-Contextual set S_{nc} and its Complement* S_c

$$H = H_{nc} + H_c$$

1. Run the Classical simulation of the noncontextual (H_{nc}) VQE and obtain the first part of the approximation.

2. Compute correction to the Classical result by running VQE on the remaining part H_c of H on an ansatze that corresponds to the ground state of the noncontextual part.

* doesn't neccessarily make S_c contextual

Step-1: The Non-Contextual Simulation

$$S_{nc}$$

$$\Downarrow$$

$$\mathcal{R} \equiv \{C_{i1} \mid i = 1, 2, \ldots, N\} \cup G$$

$$\Downarrow$$

$v_i \in \{\pm 1\}^{|R|} \equiv$ Ontic States

$$\Downarrow$$

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

$$\Downarrow$$

$\langle H \rangle_{(\vec{q},\vec{r})} = \sum_{B \in \overline{G}} \left(h_B + \sum_{i=1}^{N} h_{B,i} r_i\right) \prod_{j \in \mathcal{J}_B} q_j \longleftarrow$ Minimize this to get the ground state energy

Meaning of Epistemic states (quasi-quantised states)

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

$$\mathcal{R} \equiv \{C_{i1} \mid i = 1, 2, \dots, N\} \cup G$$

In terms of $(\vec{q}, \vec{r})$, the expectation values for $\mathcal{R}$ are

$$\langle G_j \rangle_{(\vec{q},\vec{r})} = q_j,$$

$$\langle C_{i1} \rangle_{(\vec{q},\vec{r})} = r_i.$$

Define $A = \sum_i r_i C_{i1}$ where $|\vec{r}| = 1$, $q_j \in \{\pm 1\}$

$$\Downarrow$$

$< A >_{\vec{q},\vec{r}} = 1$ & $< G_j >_{\vec{q},\vec{r}} = q_j$

This means that each $(\vec{q}, \vec{r})$ represents a joint eigenspace of the Observables $G \cup \{A\}$

Epistemic states $\equiv$ JointEigenspace of $G \cup \{A\}$

Before getting to step 2, we need to check if we really require it

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

$$\Downarrow$$

$$\overrightarrow{q_0}, \overrightarrow{r_0} \longleftarrow \text{Non contextual ground statespace}$$

$\overrightarrow{q_0}, \overrightarrow{r_0}$ represents joint Eigenspace of $G \cup \{A\}$

$$H = H_{nc} + H_c$$

If the non contextual states of H_{nc} uniquely identify quantum states, then for any non contextual state the expectation value of every term in H_c is zero i.e. No Quantum Correction is Possible.

Non-degeneracy of $\overrightarrow{q_0}, \overrightarrow{r_0}$ eigenspace $\Longrightarrow$ No Quantum Correction needed

Step-2 : Compute Quantum correction to the classical simulation

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

$$\Downarrow$$

$$\overrightarrow{q_0}, \overrightarrow{r_0} \longleftarrow \text{Non contextual ground statespace}$$

This Eigenspace is called the Contextual Subspace

Run a VQE for H_c on the Contextual subspace to calculate the quantum correction

Turns out that this can be done on less than n-qubits by restricting H_c to a subset of n-qubits

Restricting H_c to a subset of n-qubits

$$H = H_{nc} + H_c$$

Restriction can be done by mapping the Contextual Subspace to a Stabilizer subspace

For any Unitary U, If we map an Observable $A \rightarrow UAU^\dagger$ then:

$$< A >_{|\Psi>} = < UAU^\dagger >_{U|\Psi>}$$

Eigenvalues and hence statistics of A are preserved under Unitary Transformation.

Restricting H_c to a subset of n-qubits

$$H = H_{nc} + H_c$$

It is possible to construct a Unitary D that takes $H \to DHD^\dagger$ such that

$$G_j \to Z^k = DG_jD^\dagger$$

i.e. each of the operators in G get mapped to some single Qubit Pauli $Z^k = I_1 \otimes \ldots \otimes Z_k \ldots \otimes I_n$.

$$\mathcal{R} \equiv \{C_{i1} \mid i = 1, 2, \ldots, N\} \cup G$$

Since R is an independent set of operators with G being a set of independent Casimirs and $G \cup \{C_{i1}\}$ also forms an Independent Commuting set, Therefore $|G| \leq n - 1$.
(Because n-qubit system can only have n Independent Commuting Operators at max.)

Therefore under Unitary D, set G gets mapped to Single Qubit Pauli's which require atmost $|G|$ qubits.

Restricting H_c to a subset of n-qubits

Let $\mathscr{H}_1$ denote the Hilbert space of $|G| = n_1$ qubits acted on by single-qubit Pauli Z operators, and let $\mathscr{H}_2$ denote the Hilbert space of remaining n_2 qubits s.t. $n = n_1 + n_2$ with $\mathscr{H}_n = \mathscr{H}_1 \otimes \mathscr{H}_2$.

Under Unitary D, $H_c \rightarrow DH_cD^\dagger = H_c^{'}$

Therefore $H_c^{'} = \sum_P h_p P$

where $P = P_1 \otimes P_2 = (P_1 \otimes I)(I \otimes P_2)$

Further it can be shown that $P|\Psi(\overrightarrow{q_0}, \overrightarrow{r_0}) > = p_1 h_P (I \otimes P_2)|\Psi(\overrightarrow{q_0}, \overrightarrow{r_0}) >$

$p_1 = \pm 1$

Hence, effectively $H_c^{'}$ acts only on the n_2 qubits.

Perform VQE for $H_c^{'}$ on $n_2 < n$ qubits to attain the quantum correction.

This would complete the CS-VQE implementation!!!

Summary

- What are VQAs? Why we need them? (Dis)Advantages? Open Problems?
- What Constitutes a test of Contextuality for VQEs?
- Classical Simulation for Hamiltonians failing this test.
- Combining the Classical simulation with VQE to produce another hybrid-algorithm.

Thank you!!!

Any Questions???