Title: Variational Quantum Eigensolvers and contextuality

Speakers: Peter Love

Collection: Symmetry, Phases of Matter, and Resources in Quantum Computing

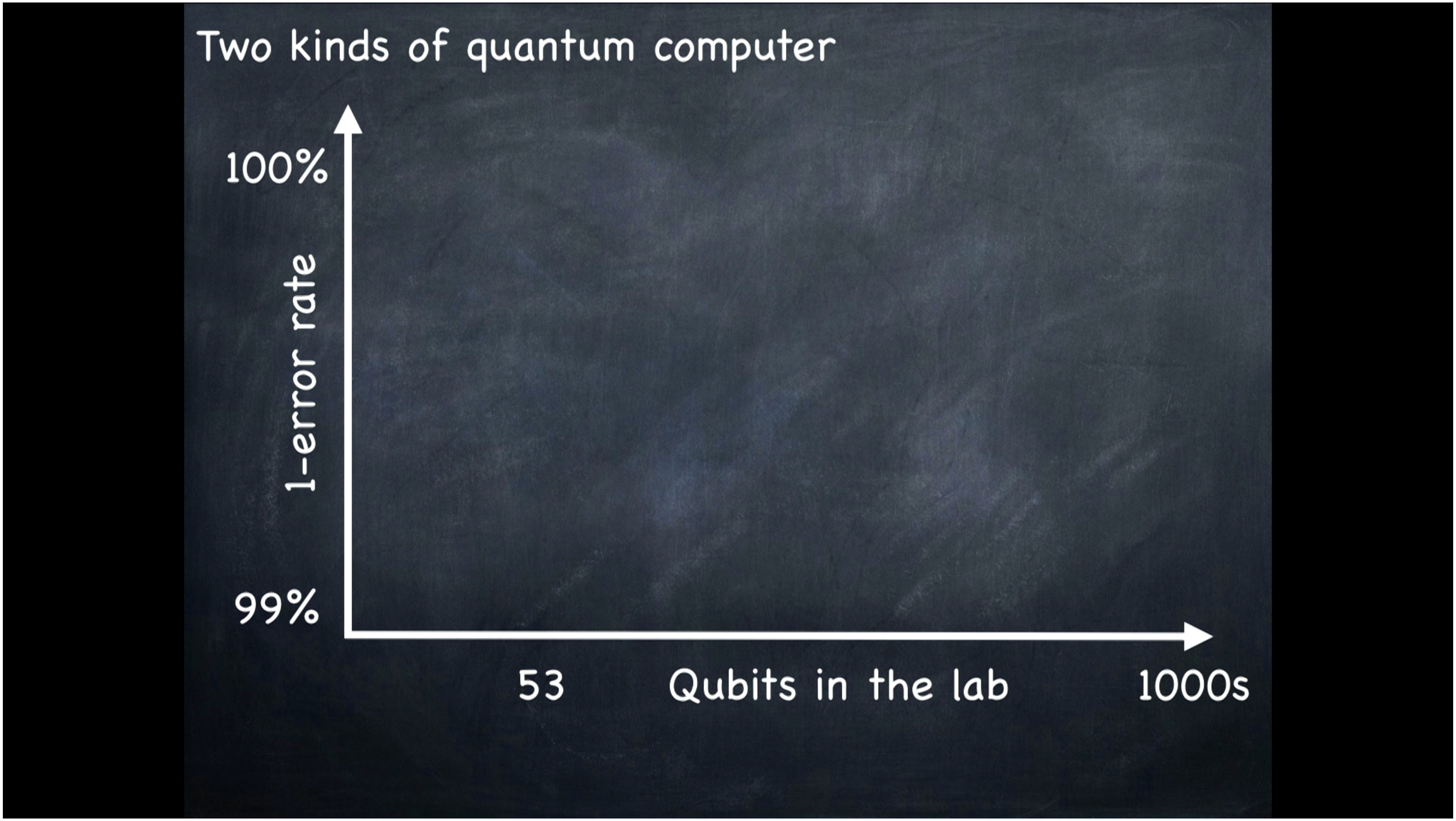
Date: November 26, 2019 - 3:30 PM

URL: http://pirsa.org/19110121

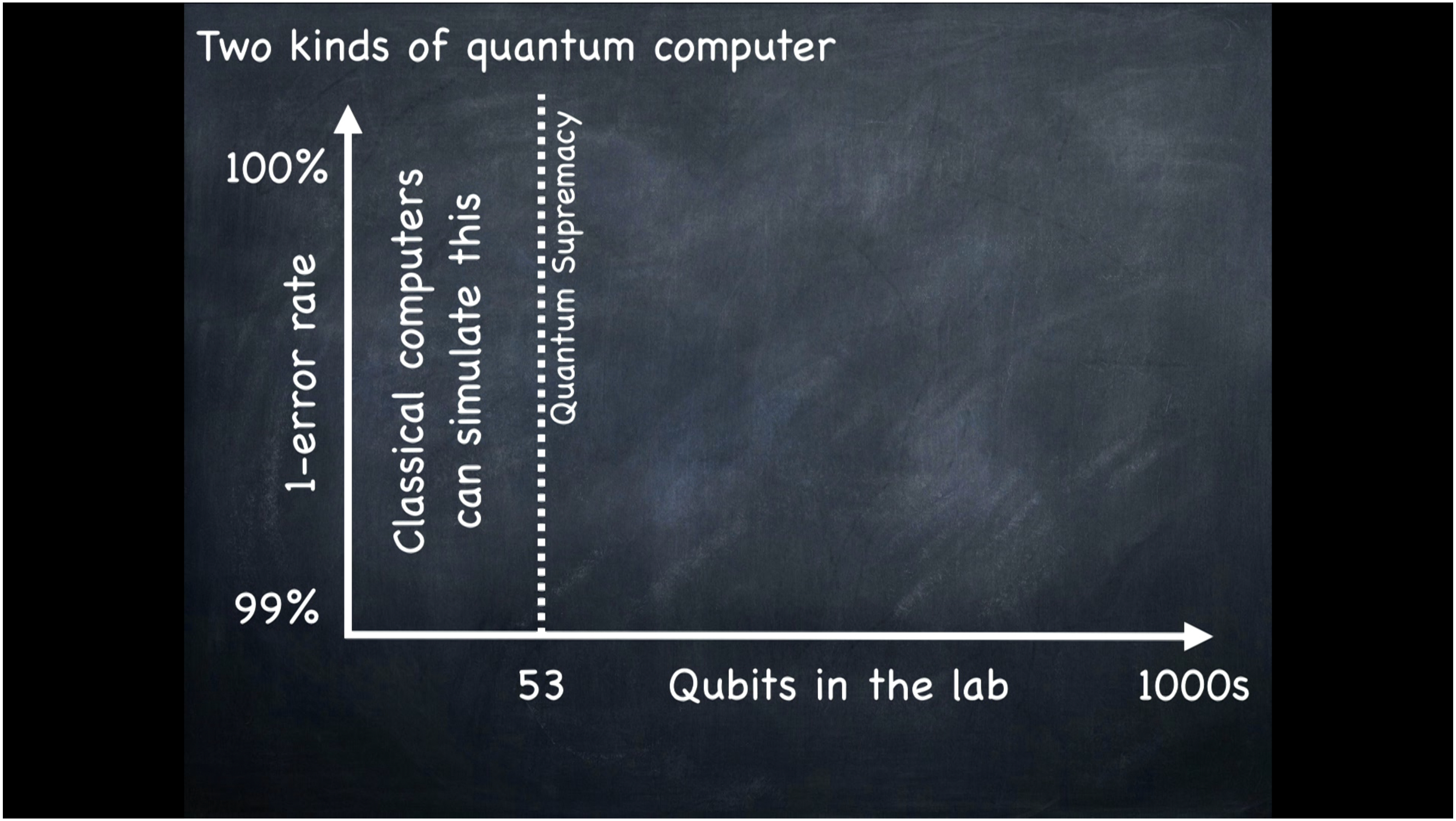
Abstract: The variational quantum eigensolver (VQE) is the leading candidate for practical applications of Noisy Intermediate Scale Quantum (NISQ) devices. The method has been widely implemented on small NISQ machines in both superconducting and ion trap implementations. I will review progress to date and discuss two questions . Firstly, how quantum mechanical are small VQE demonstrations? We will analyze this question using strong measurement contextuality. Secondly, can VQE be implemented at the scale of devices capable of exhibiting quantum supremacy, around 50 qubits? I will discuss some recent techniques to reduce the number of measurements required, which again use the concept of contextuality.

Variational Quantum Eigensolvers and Contextuality

Peter Love
Department of Physics and Astronomy
Tufts University
and Brookhaven National Lab



Two kinds of quantum computer
100%
1-error rate
99%
53
Qubits in the lab
1000s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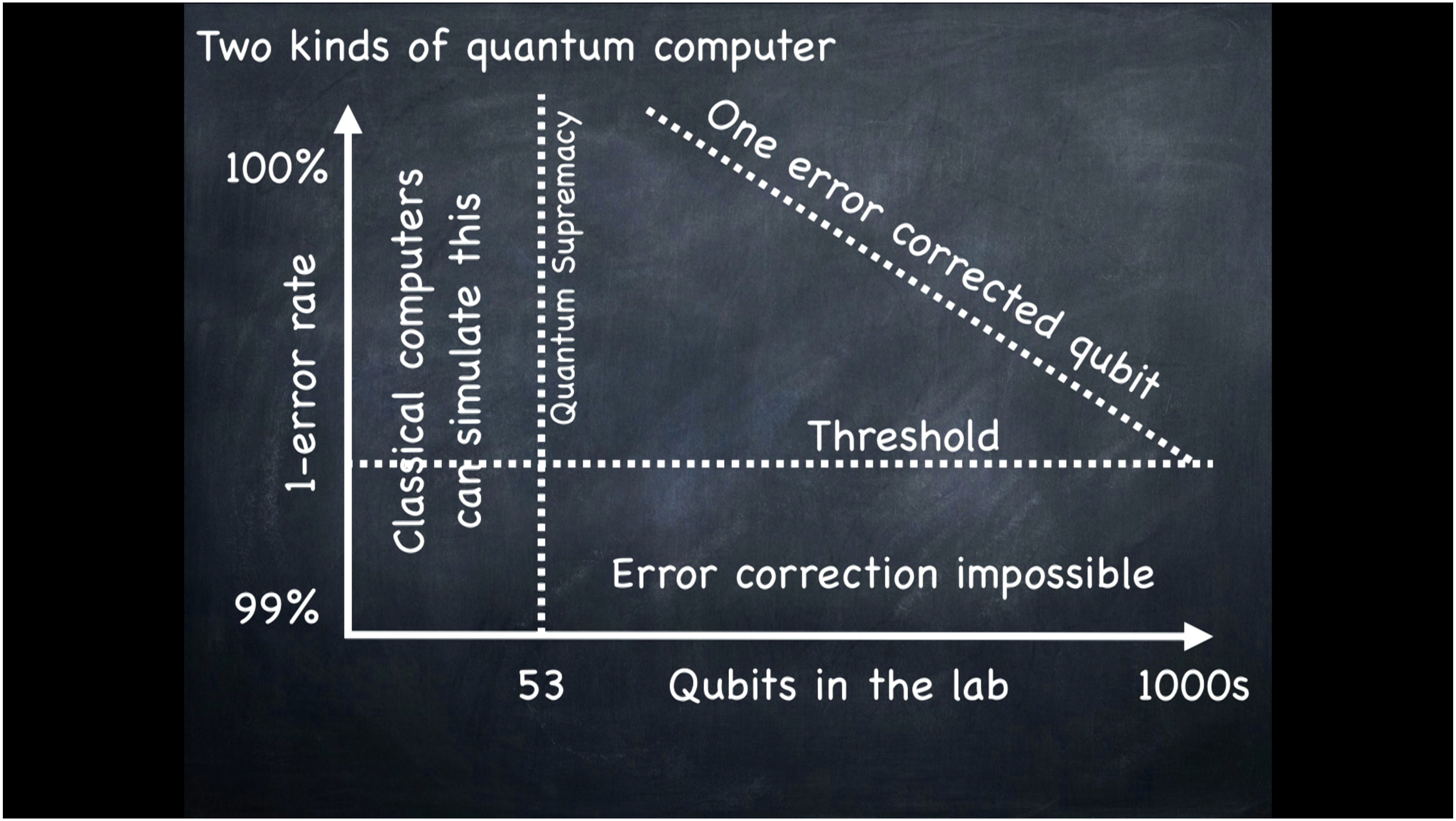
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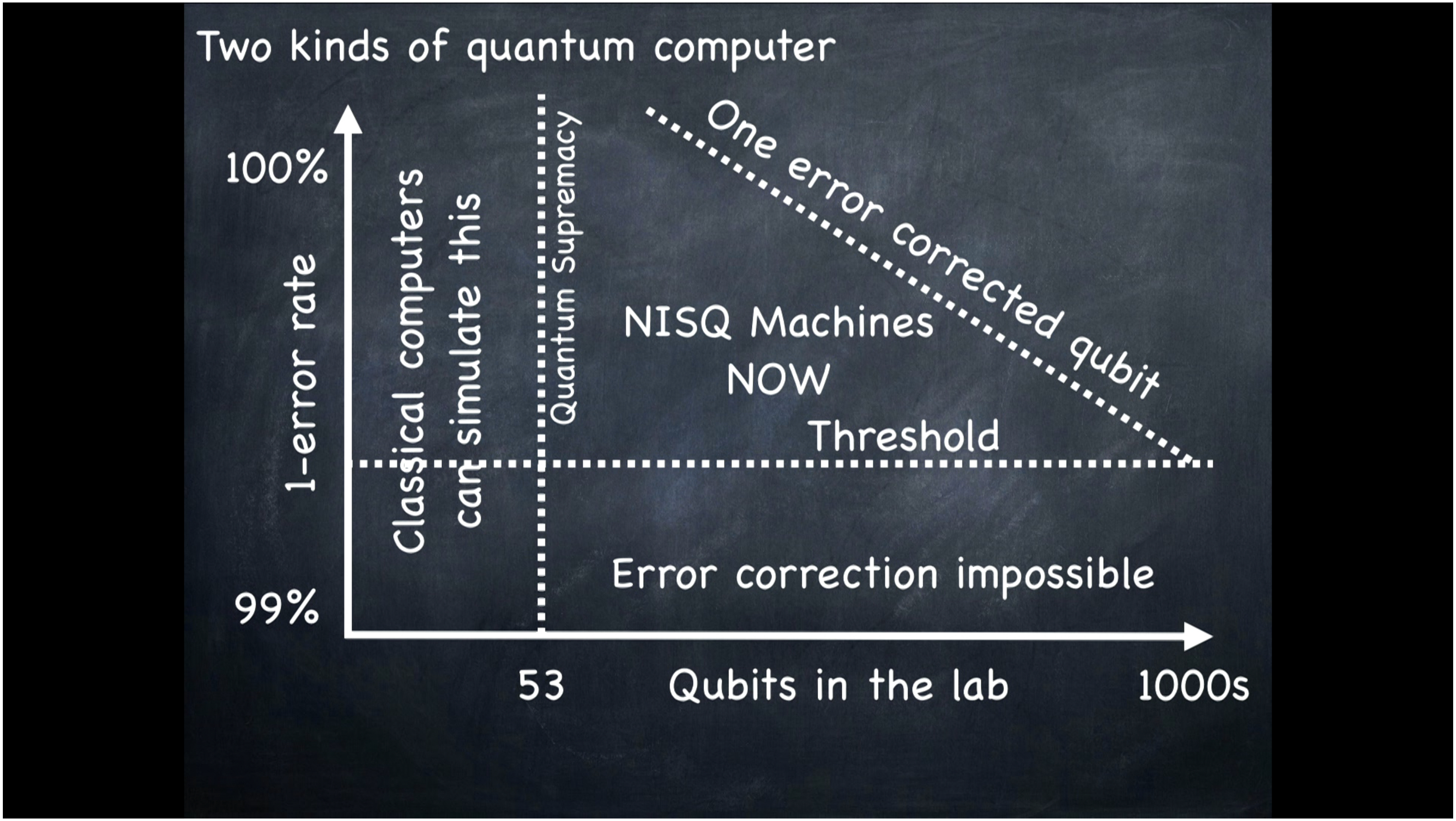
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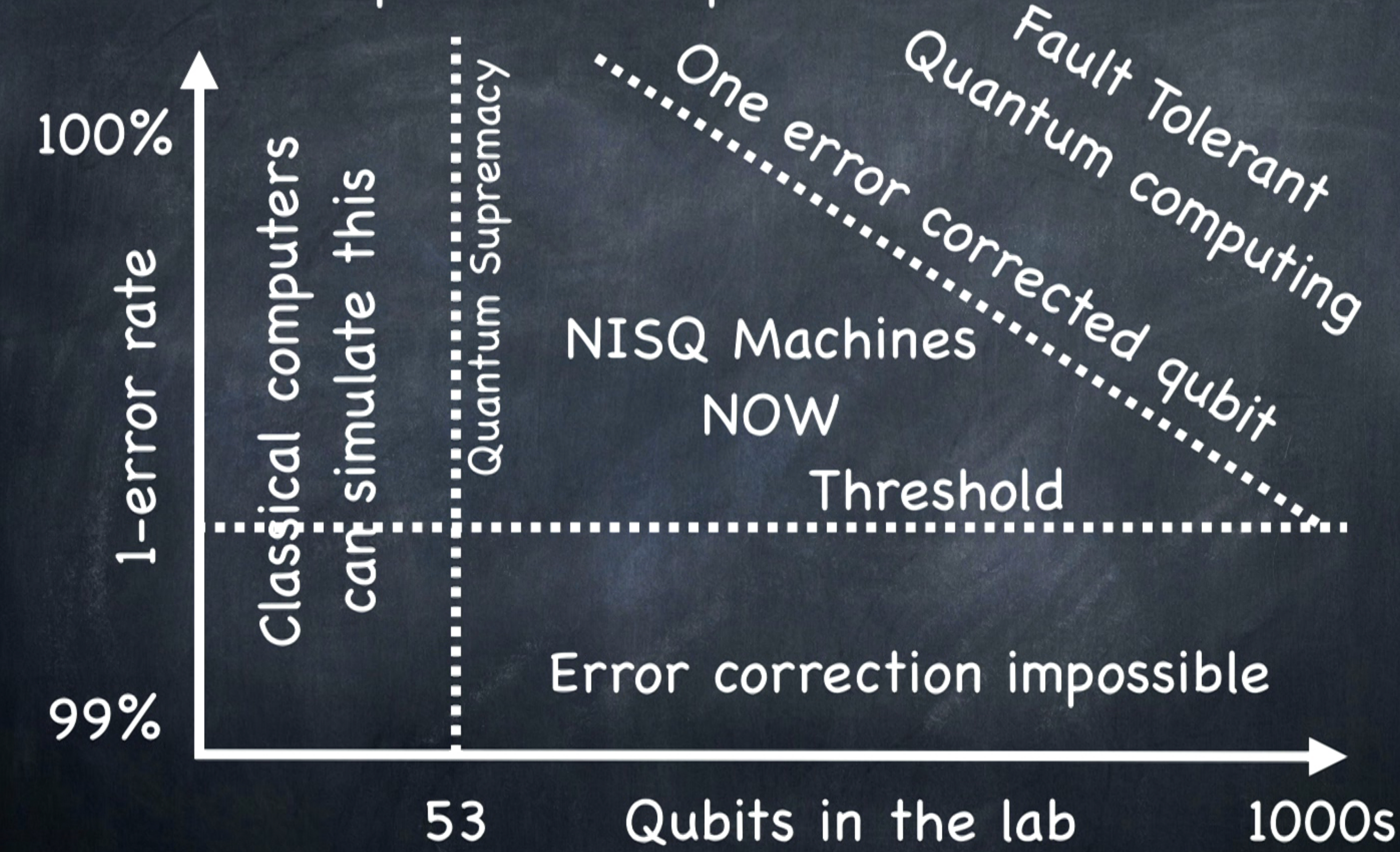
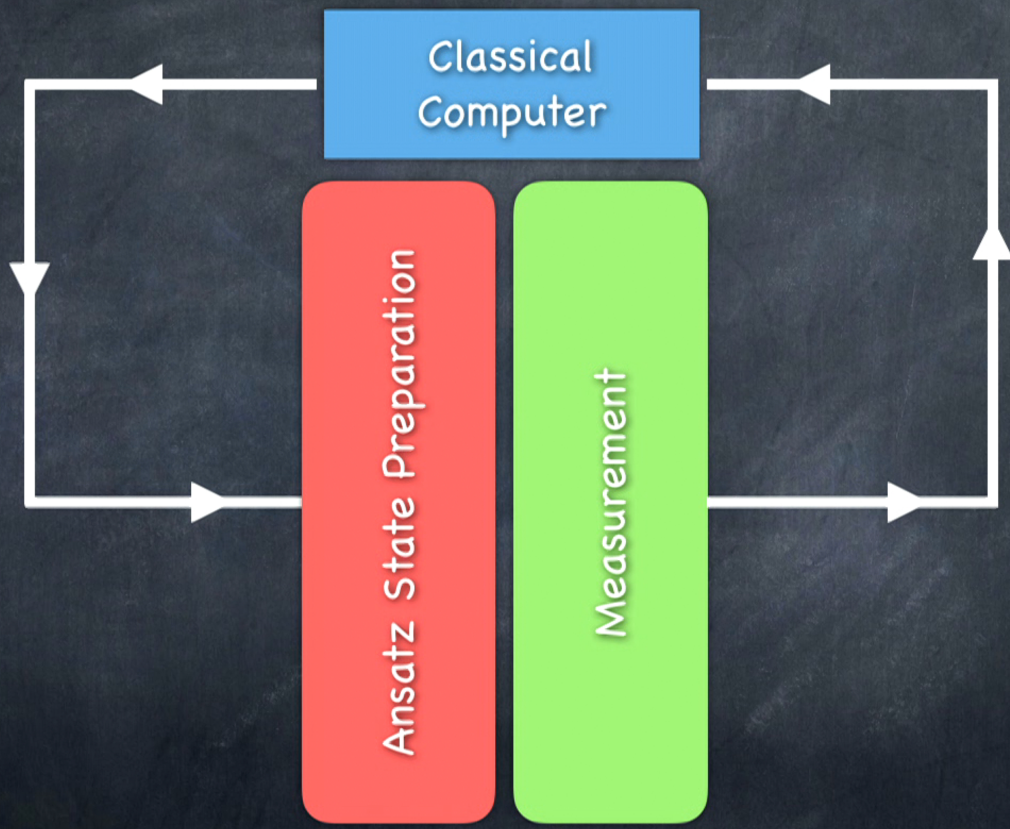
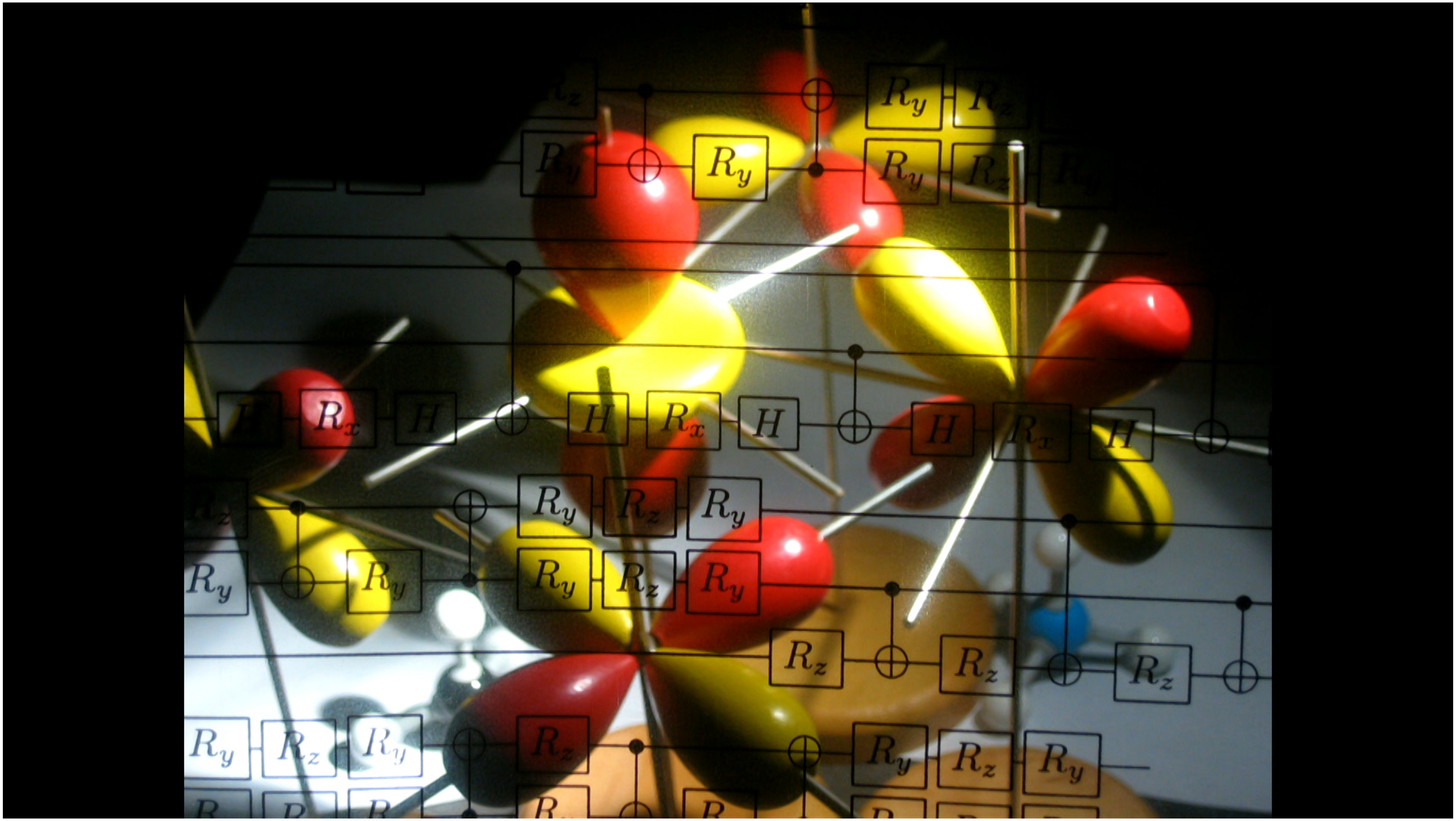


Variational NISQ algorithms




R_y R_z
R_y R_y R_z
H R_x H H R_x H H R_x H
R_y R_z R_y
R_y R_y R_y R_z R_y
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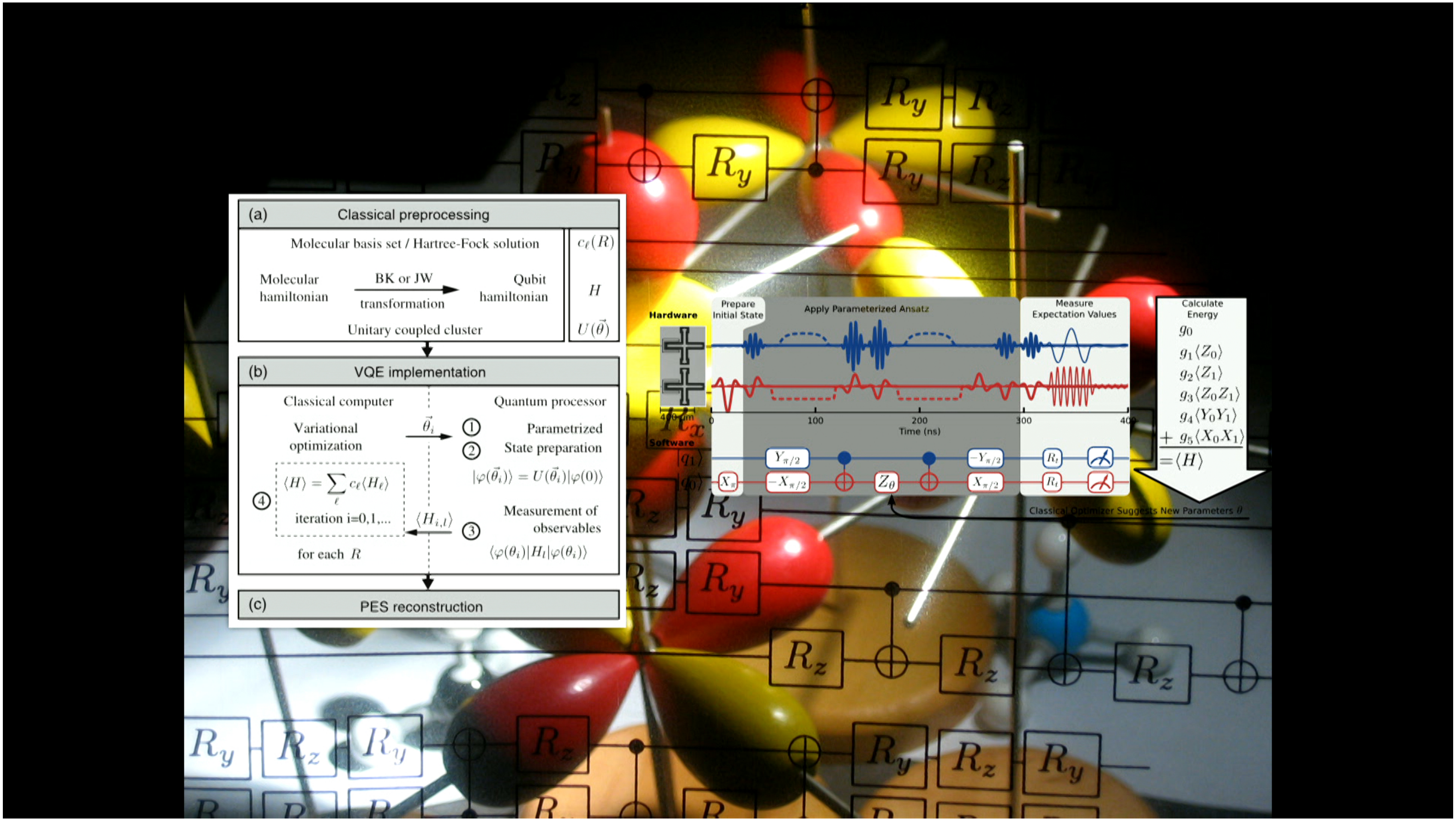
R_y R_z R_y R_z R_y R_z R_y


(a) Classical preprocessing
Molecular basis set / Hartree-Fock solution
Molecular hamiltonian
BK or JW transformation
Qubit hamiltonian
Unitary coupled cluster
$c_\ell(R)$
H
$U(\vec{\theta})$
(b) VQE implementation
Classical computer
Quantum processor
Variational optimization
$\vec{\theta}_i$
① Parametrized
② State preparation
$|\varphi(\vec{\theta}_i)\rangle = U(\vec{\theta}_i)|\varphi(0)\rangle$
④ $\langle H \rangle = \sum_\ell c_\ell \langle H_\ell \rangle$
iteration i=0,1,...
$\langle H_{i,l} \rangle$
③ Measurement of observables
$\langle \varphi(\theta_i)|H_l|\varphi(\theta_i)\rangle$
for each R
(c) PES reconstruction
Hardware
Software
Prepare Initial State
Apply Parameterized Ansatz
Measure Expectation Values
Calculate Energy
Time (ns)
g_0
$g_1\langle Z_0 \rangle$
$g_2\langle Z_1 \rangle$
$g_3\langle Z_0 Z_1 \rangle$
$g_4\langle Y_0 Y_1 \rangle$
$+\ g_5\langle X_0 X_1 \rangle$
$= \langle H \rangle$
Classical Optimizer Suggests New Parameters θ

Variational Quantum Eigensolver - VQE

We want to find the smallest eigenvalue of:

$$H = \sum_{P_i \in S} \alpha_i P_i$$

Variationally minimize:

$$\langle H \rangle = \sum_{P_i \in S} \alpha_i \langle P_i \rangle$$

A variational eigenvalue solver on a quantum processor Peruzzo, et al Nature communications 5 (4213), (2014),
Scalable Quantum Simulation of Molecular Energies, O'Malley et al. Physical Review X 6 (3), 031007,
Quantum chemistry calculations on a trapped-ion quantum simulator, Hempel et al, http://arxiv.org/abs/1803.10238

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Classically separate minimization of each term fails - rdms do not correspond to global state

Quantumly one can variationally minimize a global quantum state, evaluate terms separately

A variational eigenvalue solver on a quantum processor Peruzzo, et al Nature communications 5 (4213), (2014),
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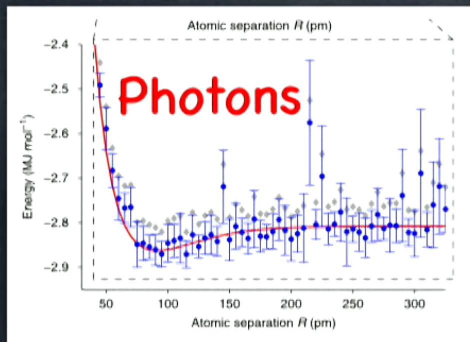
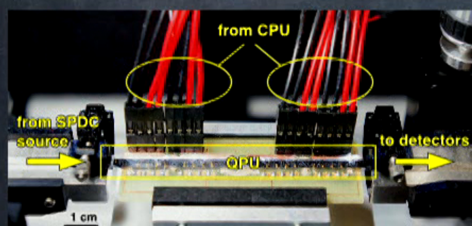
Quantum chemistry calculations on a trapped-ion quantum simulator, Hempel et al, http://arxiv.org/abs/1803.10238

Nasty, brutish and short: VQE on NISQ devices





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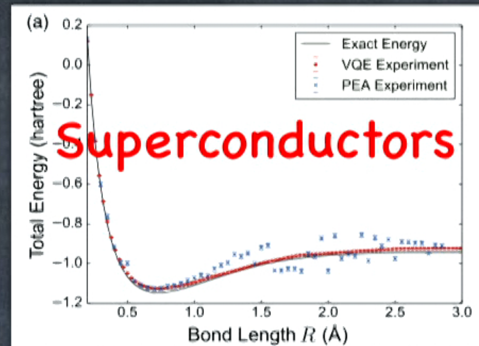

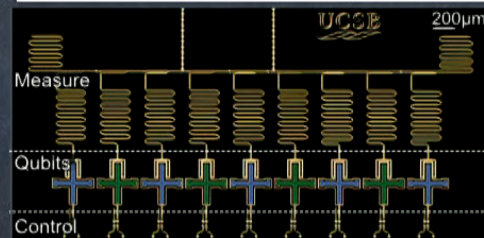

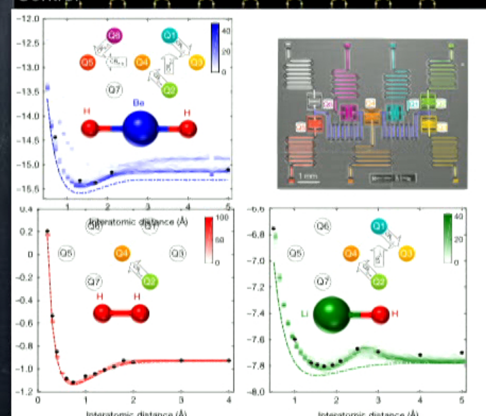

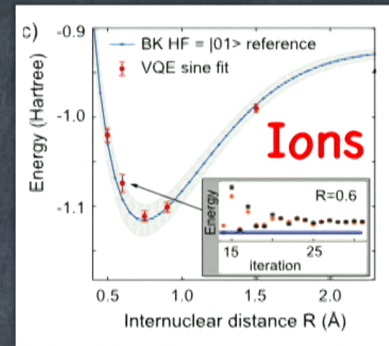

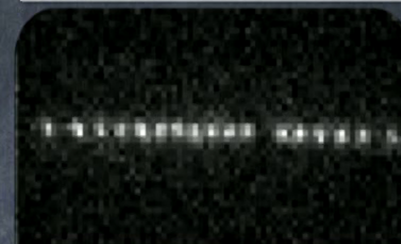

Quantum chemistry calculations on a trapped-ion quantum simulator, Hempel et al, Phys. Rev. X 8, 031022 (2018)

Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets, Kandala et al., Nature 549, pages 242–246 (2017)

Quantum Approximate Optimization Algorithm -QAOA

Restrict H to encode a classical combinatorial optimization problem and maximize. E.g.:

$$\frac{1}{2}\langle\psi|\sum_{E\in G}(1-ZZ_E)|\psi\rangle$$

Restrict ansatz to be generated by rounds of two operations:

A Quantum Approximate Optimization Algorithm Edward Farhi, Jeffrey Goldstone, Sam Gutmann
https://arxiv.org/abs/1411.4028

Quantum Approximate Optimization Algorithm -QAOA

Restrict H to encode a classical combinatorial optimization problem and maximize. E.g.:

$$\frac{1}{2}\left\langle\psi\left|\sum_{E\in G}(1-ZZ_E)\right|\psi\right\rangle$$

Restrict ansatz to be generated by rounds of two operations:

$$\prod_{E\in G} e^{-i\theta_E C_E} \qquad \prod_{V\in G} e^{-i\theta_V X}$$

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Can they achieve quantum advantage?

- Next decade should settle that

Only consider measurements - when can the outcomes be preassigned?

Set of terms: $S = \{P_i\}$

Hamiltonian: $H = \sum_{P_i \in S} \alpha_i P_i$

Only consider measurements - when can the outcomes be preassigned?

Assignment: $a : i \longrightarrow \pm 1$

Set of terms: $S = \left\{ P_i \right\}$

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Only consider measurements - when can the outcomes be preassigned?

Inference: Any product from an abelian subset of S can be inferred from a.

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Only consider measurements - when can the outcomes be preassigned?

Closure of S under inference: smallest closed subtheory including S. (Karanji et al arXiv: 1802.07744) $\bar{S}$

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Assignment: $a : i \longrightarrow \pm 1$

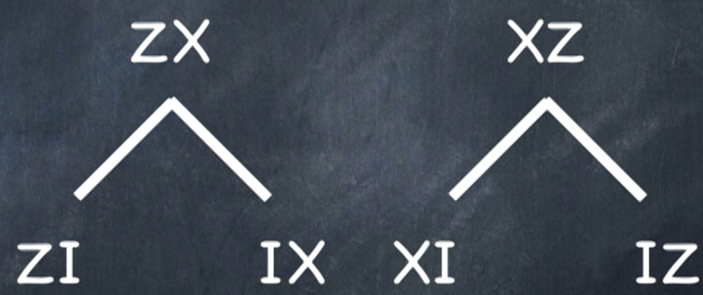
Set of terms: $S = \{P_i\}$

Hamiltonian: $H = \sum_{P_i \in S} \alpha_i P_i$

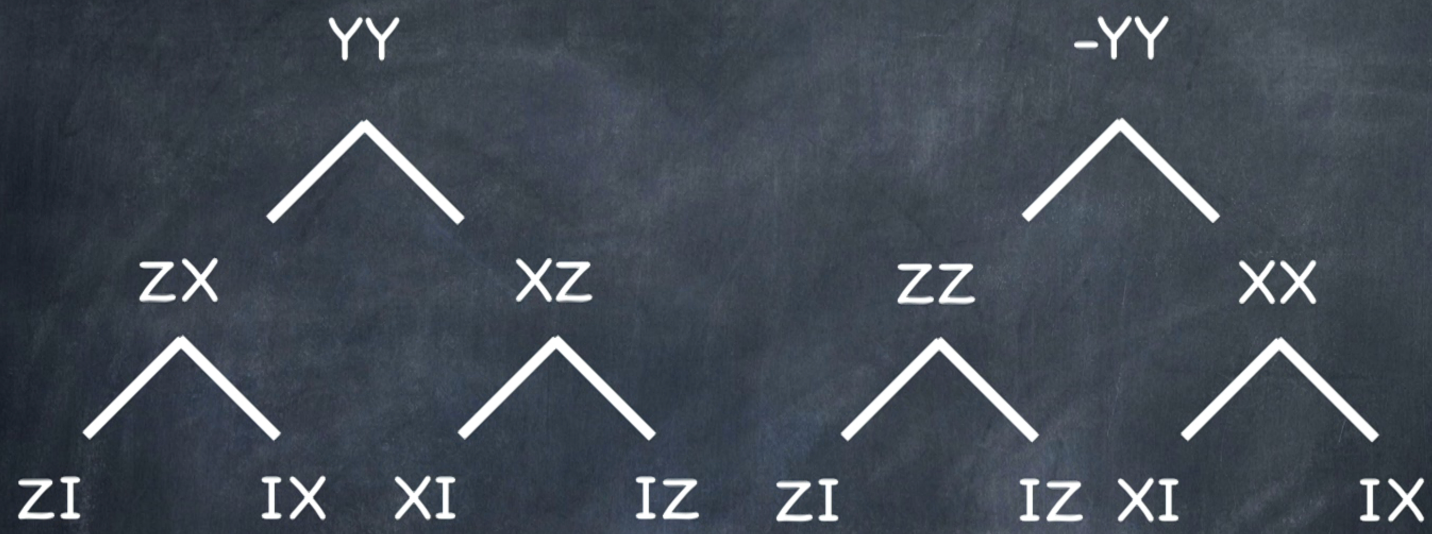
Determining trees: When is an operator in $\bar{S}$?

Parents are the
product of their children

Children of given
parent commute



Determining trees are not unique.



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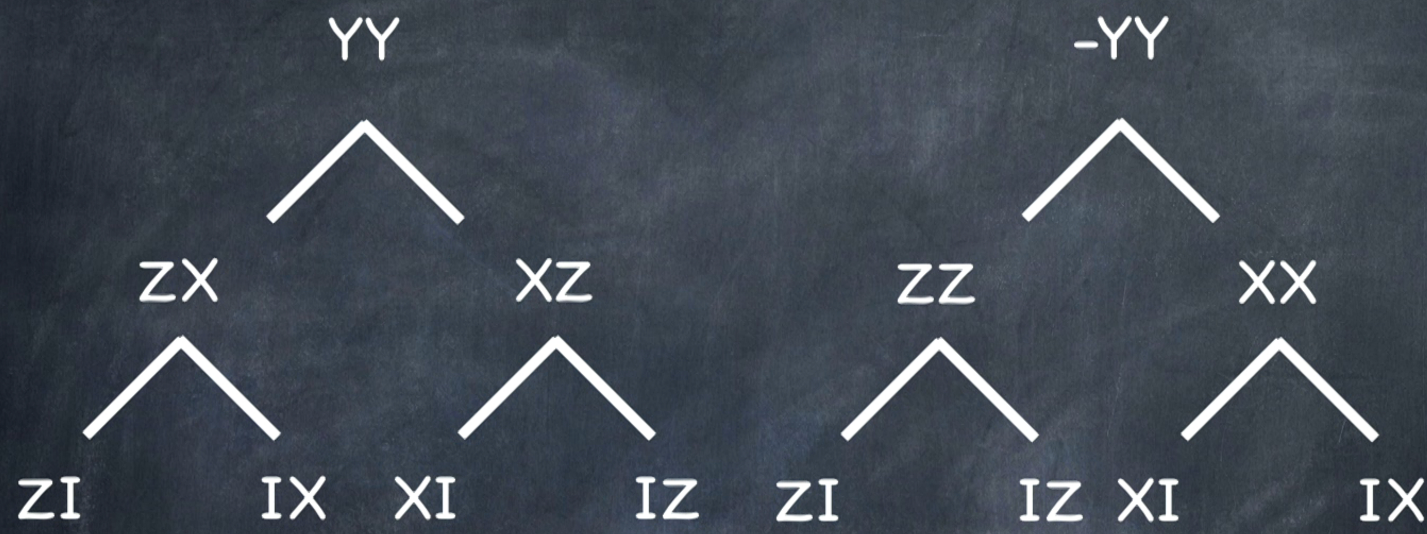

Impossible to assign values to {ZZ,XX,ZX,XZ} without contradiction -
the Peres-Mermin square obstacle.

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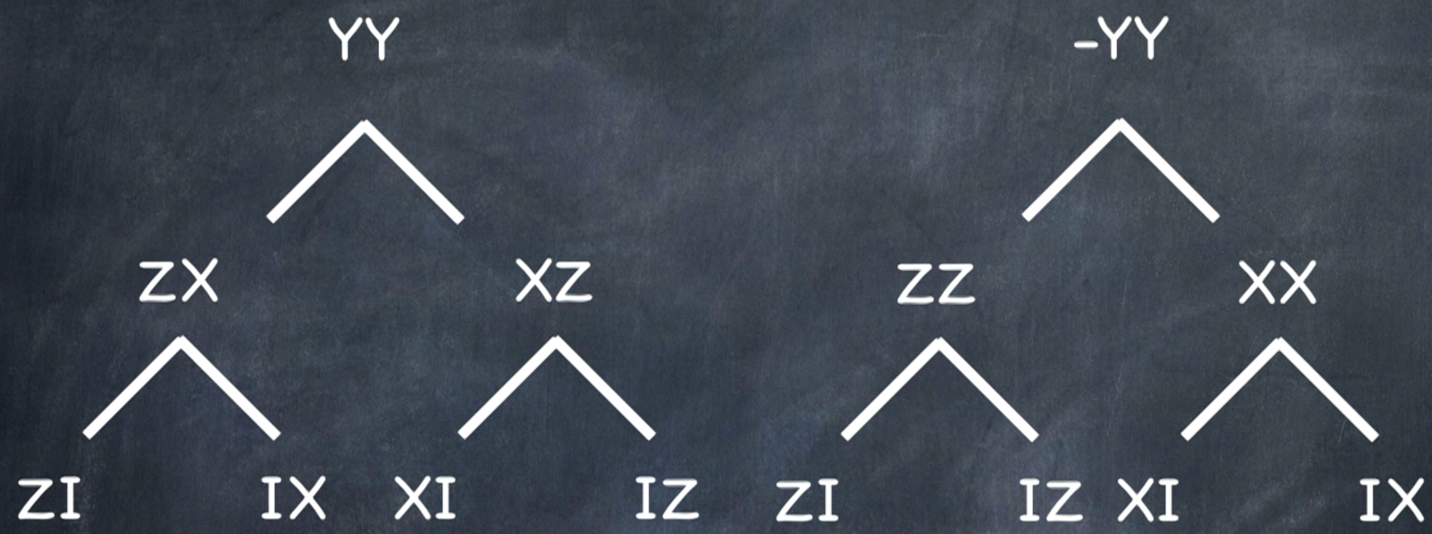
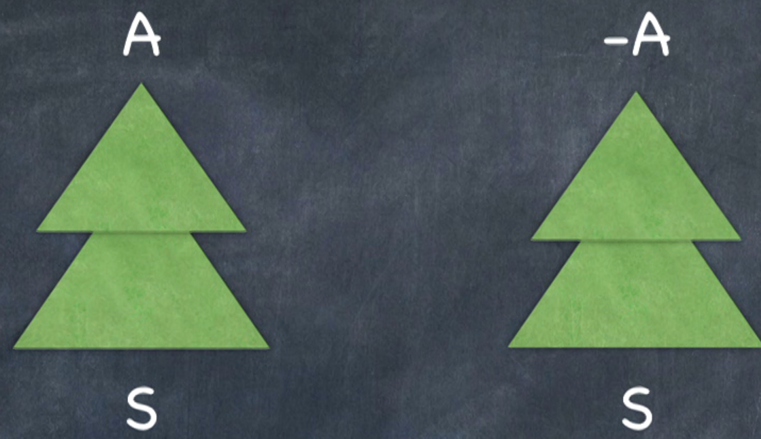


Impossible to assign values to {ZZ,XX,ZX,XZ} without contradiction
the Peres-Mermin square obstacle.

Any set S is contextual if one can write a determining tree for A and for -A, for some A.

Contextual and non-contextual S



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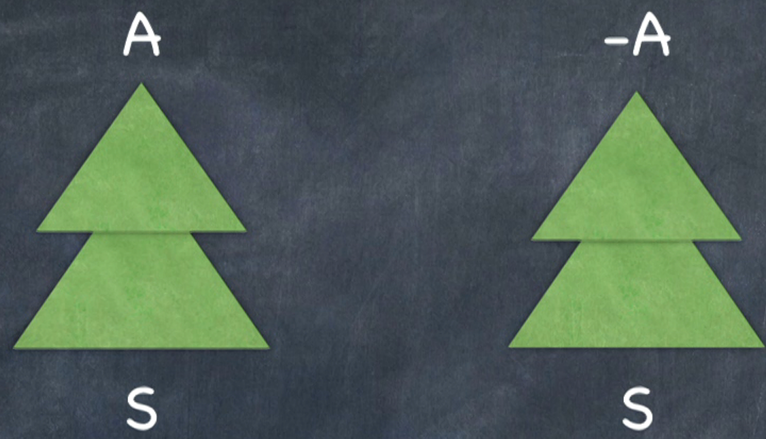

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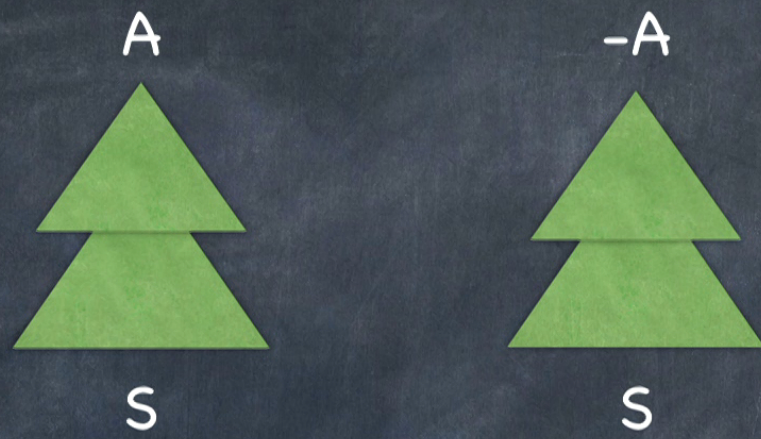
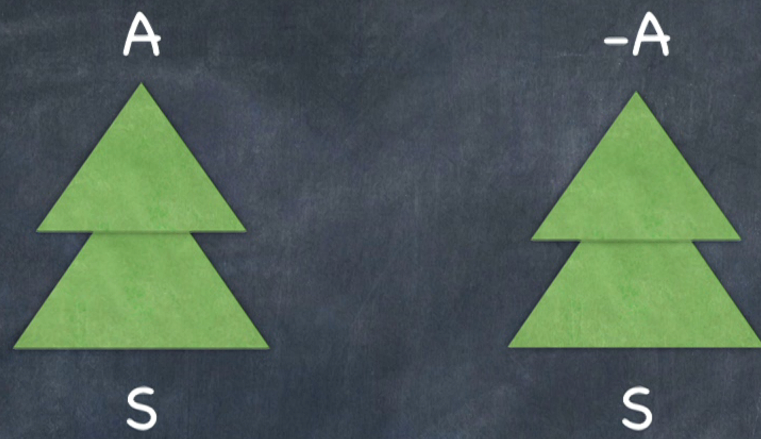


Any set S is contextual if one can write a determining tree for A and for -A, for some A.

In this case there is an operator in S itself that shows the contradiction.

Contextual and non-contextual S

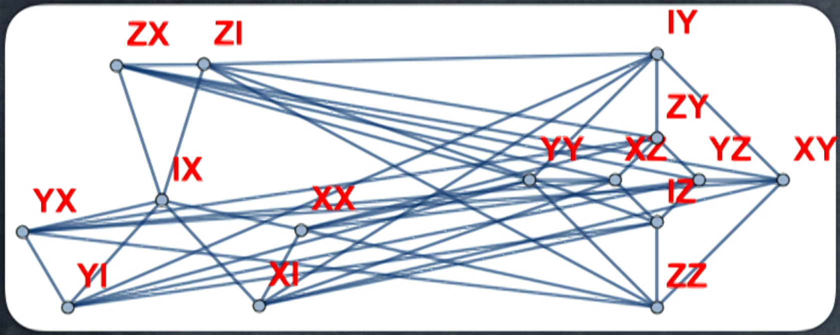


Any set S is contextual if one can write a determining tree for A and for -A, for some A.

In this case there is an operator in S itself that shows the contradiction.

How do we determine this without drawing a forest of determining trees?

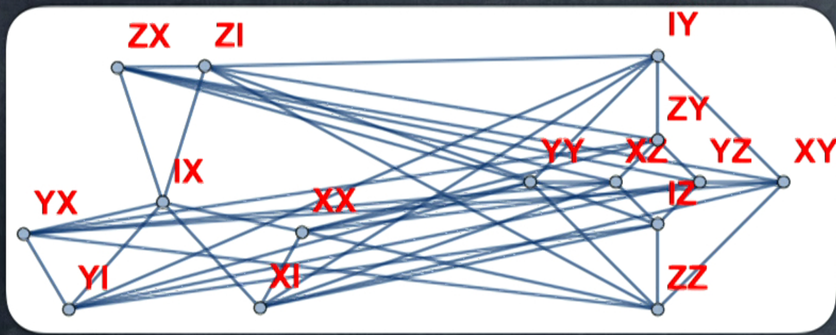
Compatibility Graph



Vertices are operators
v -> P_v

An edge (v,w) is present IFF
$[P_v, P_w] = 0$.

Compatibility Graph



Vertices are operators
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An edge (v,w) is present IFF
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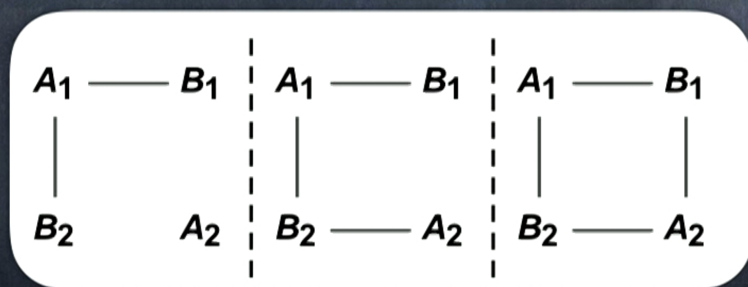
S is noncontextual if the compatibility graph lacks these subgraphs



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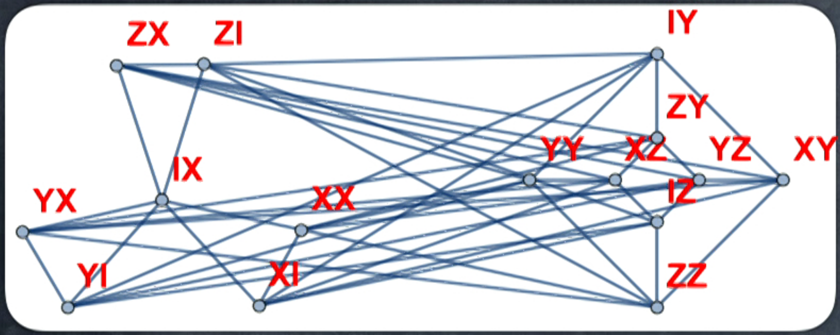

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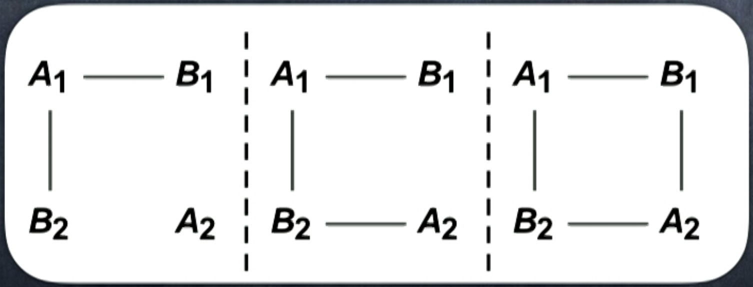

See also R. Raussendorf, J. Bermejo-Vega, E. Tyhurst, C. Okay, and M. Zurel, arXiv 1905.05374

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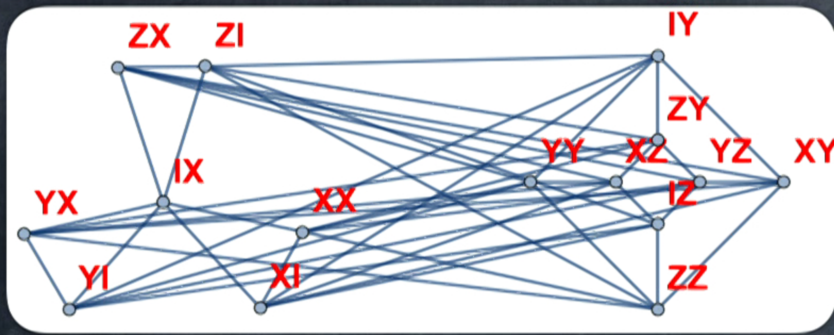

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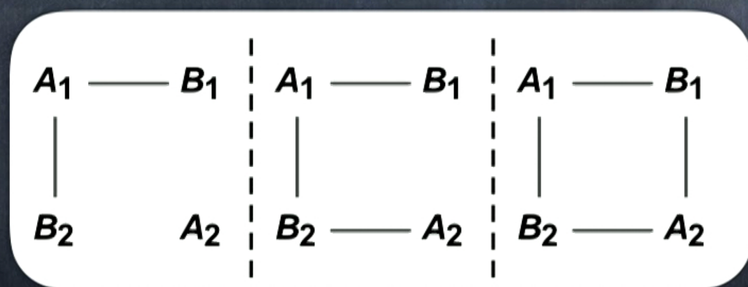


Equivalently if commutation is an equivalence relation on the compatibility graph after removal of Casimirs.

See also R. Raussendorf, J. Bermejo-Vega, E. Tyhurst, C. Okay, and M. Zurel, arXiv 1905.05374

Contextuality in VQE experiments (arXiv:1904.02260 [quant-ph])

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 ($\lvert\mathcal{S}\rvert$). In [22], $\lvert\mathcal{S}\rvert$ varies.

Summary of the first part

Call a Hamiltonian noncontextual if its S is.

QAOA is obviously noncontextual in this sense, so noncontextual VQE equivalent to QAOA

There may be quantum advantage - but has to come from clever quantum ansatz for a classical problem

Work in progress: quasi-quantized algorithm for NCVQE

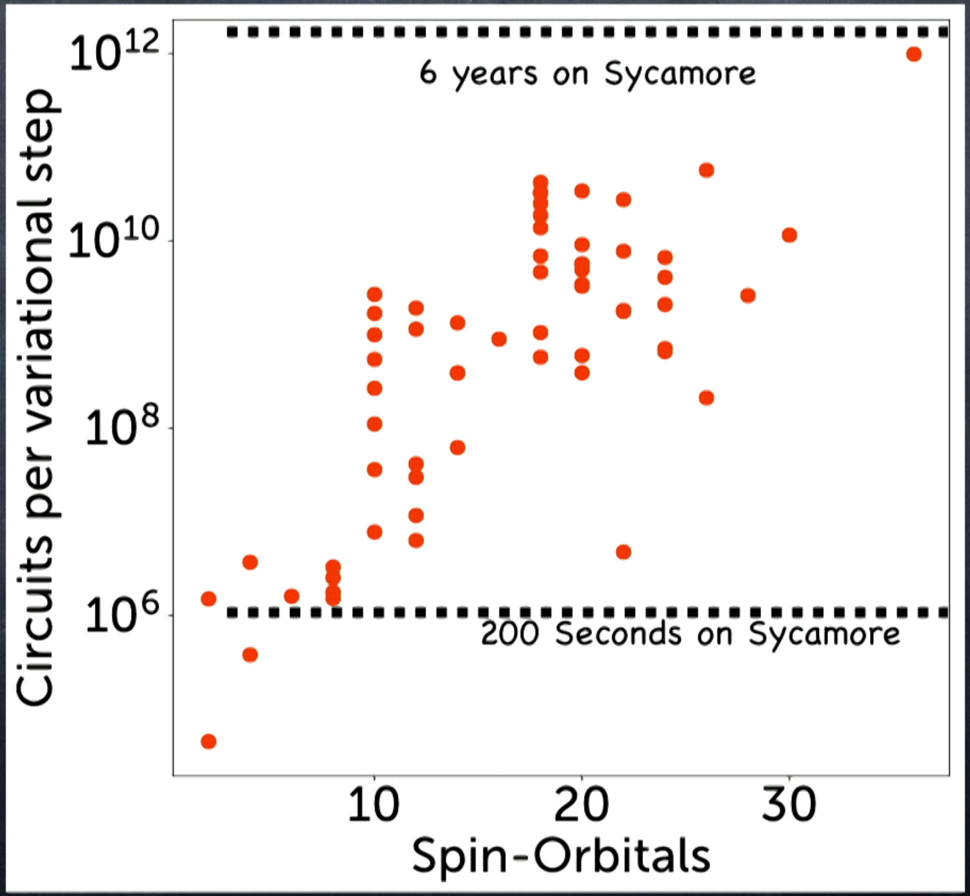
Term reduction for VQE

Problem:

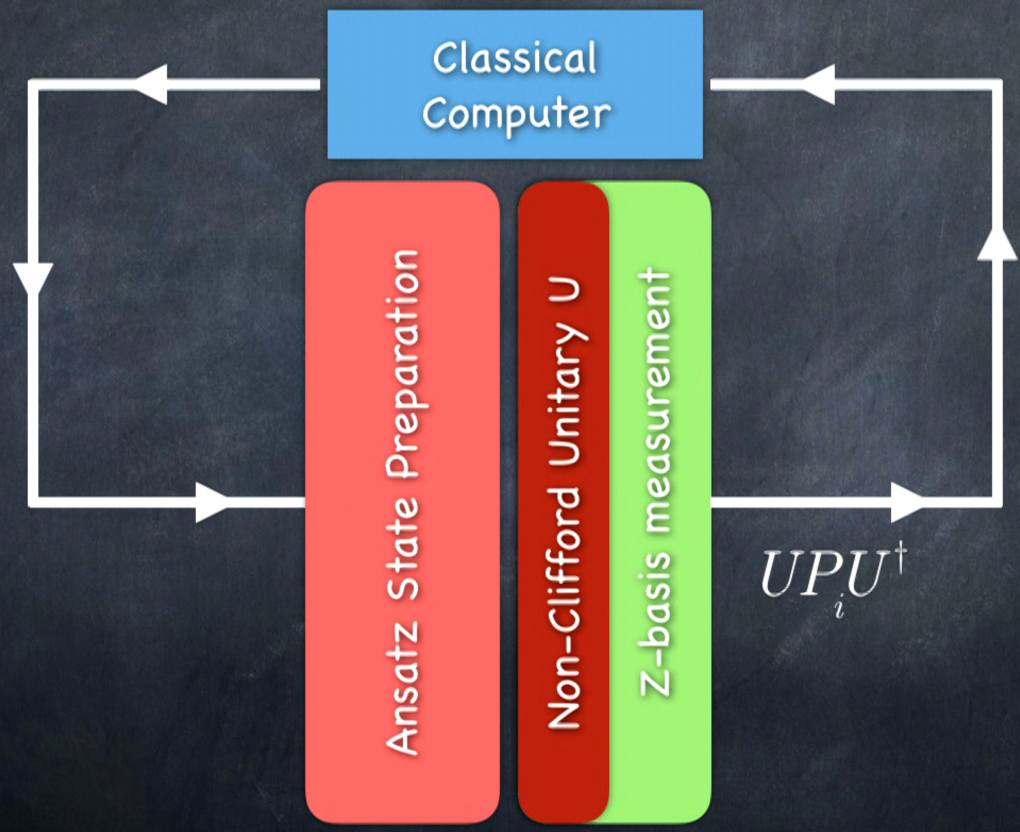
$O(N^4)$ terms in Hamiltonian

$O(1/\text{error}^2)$ repetitions

Large fixed precision reuired "Chemical accuracy"



Measurement reduction in VQE



Strategy for term reduction

Rotate a set of Paulis to a single term $$UP_kU^\dagger = \sum_j \beta_{kj} P_j$$

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Algebraic Constraint: $$\left(UP_kU^\dagger\right)^2 = \left(\sum_j \beta_{kj} P_j\right)^2 = 1$$

Implies: $$1 = \left(\sum_j \beta_{kj}^2\right) 1 + \sum_{j<l} \beta_{kj}\beta_{kl} \left\{P_j, P_k\right\}$$

Sufficient conditions: $$\sum_j \beta_{kj}^2 = 1 \qquad \left\{P_j, P_k\right\} = 0 \forall i < j$$

Strategy for term reduction

Divide Hamiltonians into sets S in which

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Strategy for term reduction

Divide Hamiltonians into sets S in which

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These are independent sets in compatibility graph

Reducing unitary can be implemented in |S| Pauli rotations.

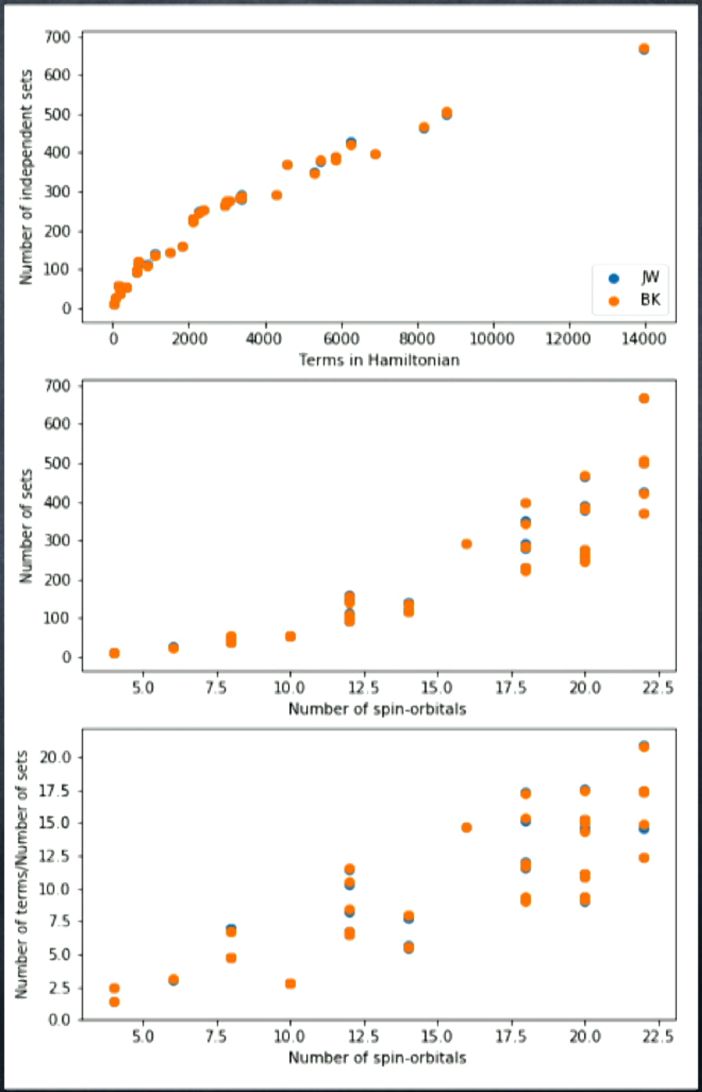
Need to find "good enough" coloring of the compatibility graph

For chemical examples on n qubits evidence suggests $|S| = O(n)$.

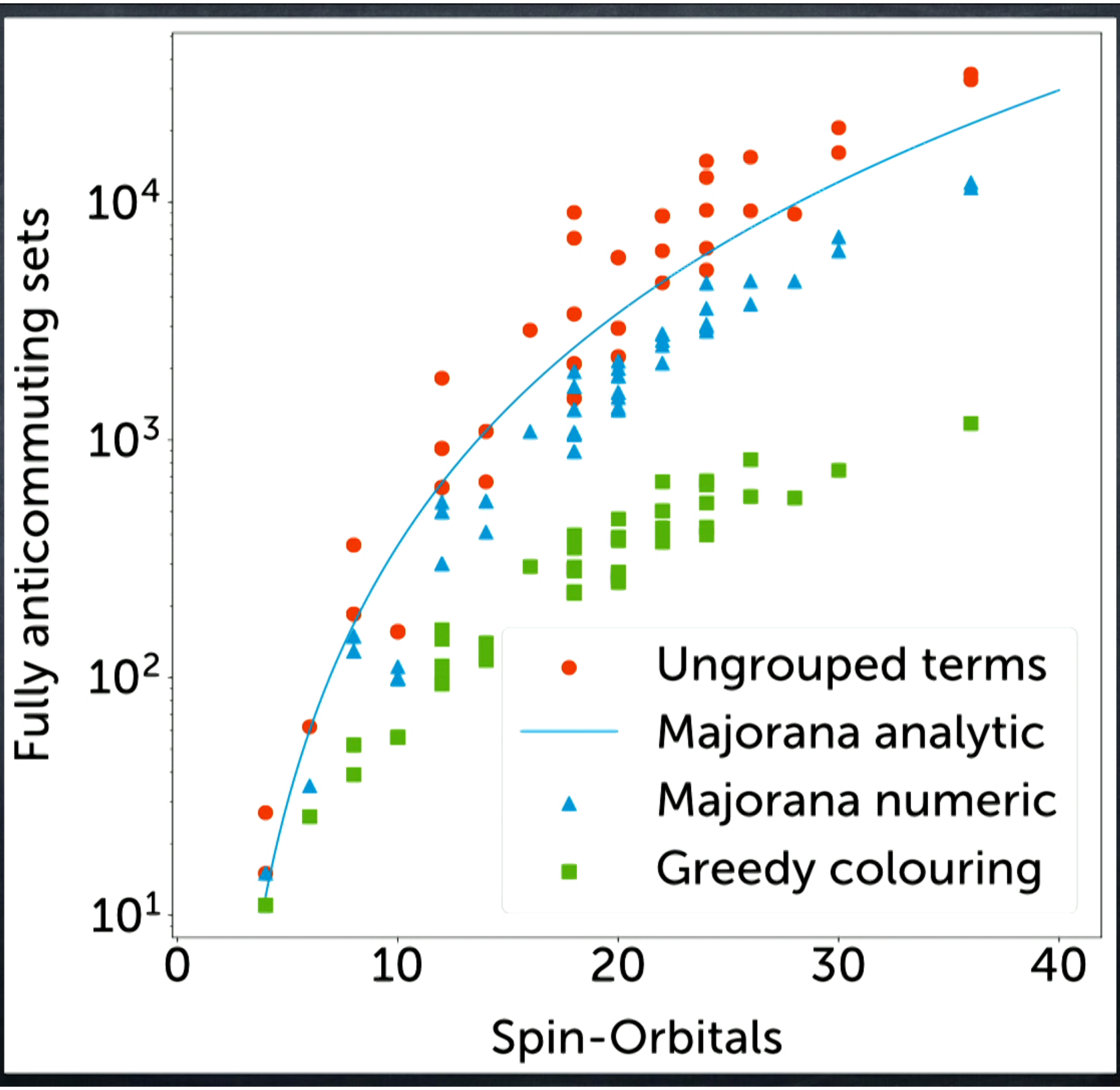
For ~ 20 qubits number of measurements reduced from 14000 to 700.

Suggests scaling reduction from n^4 to n^3

Can we establish this rigorously?

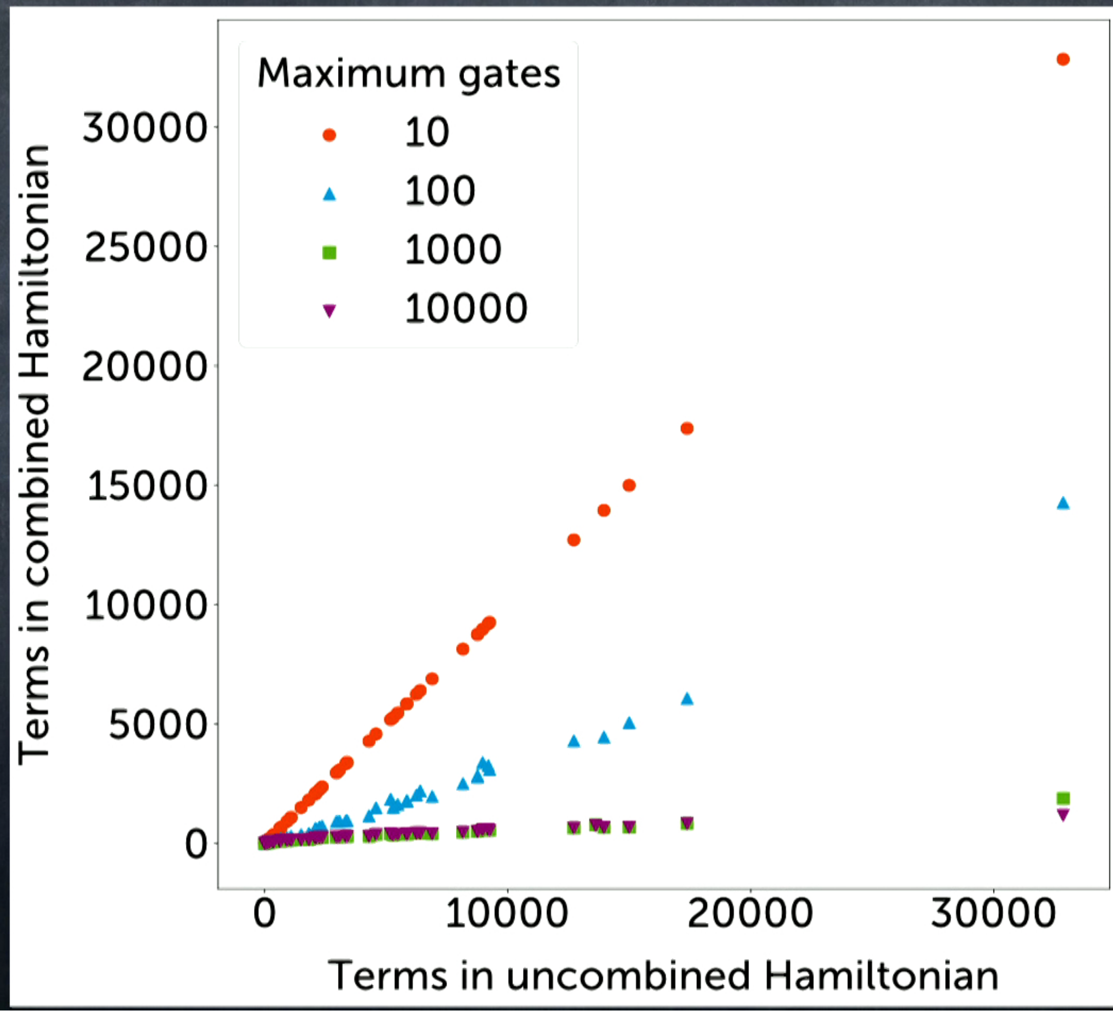


YES!



Fully anticommuting sets
10^4
10^3
10^2
10^1
0
10
20
30
40
Spin-Orbitals
Ungrouped terms
Majorana analytic
Majorana numeric
Greedy colouring

Can use whatever resources are available.



Thanks!

STAQ

arXiv:1904.02260 [quant-ph]

arXiv:1908.08067 [quant-ph]

Will Kirby	Andrew Tranter	Akimasa Miyake	Andrew Zhao