Non-contextual approximations, Magic, and Correlation energy

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QMatter Inc. (We are hiring)

From July 1: Physics & Computer Science, University of Toronto (also hiring)
with: Alexis Ralli, Tim Weaving, Sam Alterman, Basie Seibert

Quantum simulation

Map Hamiltonians of physical systems to qubit Hamiltonians

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

Pauli Hamiltonians

Generalized Pauli operators $P_i = \bigotimes_{k=1}^{n} \sigma_i^k$, e.g. $P_i = 1 \otimes Y \otimes X \ldots \otimes 1 \otimes Z$

Goal: Find ground state energy of: $H = \sum_{P_i \in S} \alpha_i P_i$ $\qquad E_0 = \min_{\vec{\theta}} \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle$

Two problems:

A) Individual $|\psi(\vec{\theta})\rangle$ may be hard to **represent** (curse of dimensionality).

B) Minimum state might be hard to **find** (e.g. classical spin glasses).

Peruzzo, Alberto, et al. "A variational eigenvalue solver on a photonic quantum processor." *Nature communications* 5.1 (2014): 1-7.

The Worst Eigensolver

Goal: Find ground state energy of: $H = \sum_{P_i \in S} \alpha_i P_i$,

$P_i^2 = 1, \quad \mathrm{spec(P_i)} = \{-1, +1\}.$

So just assign $P_i \mapsto (-1)^{b_i} \quad b_i \in \{0,1\}$, probabilistically:

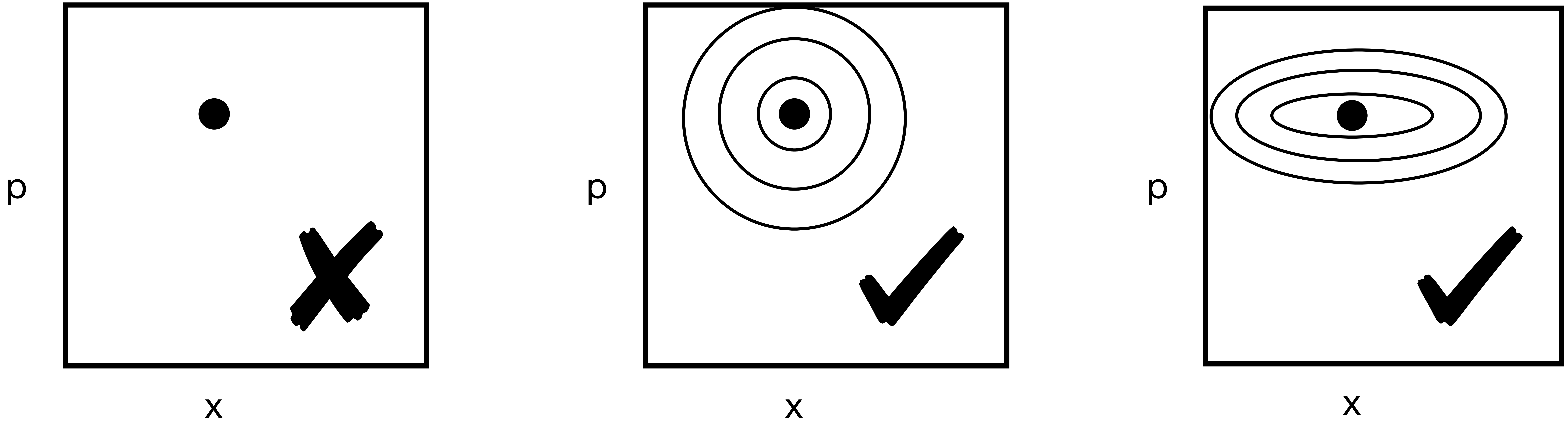
$P(b_1, b_2, \ldots, b_{|S|})$

Minimize over P.

This is a terrible idea - but why?

Peruzzo, Alberto, et al. "A variational eigenvalue solver on a photonic quantum processor." *Nature communications* 5.1 (2014): 1-7.

Obstacle: uncertainty principle



Phase points not allowed! Cannot assign definite values to non-commuting operators.

Solution: impose restrictions via probability distribution (“quasi-quantized model”)

Spekkens, Robert W. Quantum Theory: Informational Foundations and Foils (2016): 83-135.

Obstacle: Contextuality

Contextuality. Can assign values a,b to A and B if [A,B]=0.

Peres: if f(A,B)=0 for some f, then the assignments should also ensure f(a,b)=c

If $[P_a, P_b] = 0$ then assigning P_a and P_b implies assignment of $P_a P_b$

Can get contradictions in the implied assignments by choosing different commuting sets - different contexts!

Example: Kochen-Specker paradox.

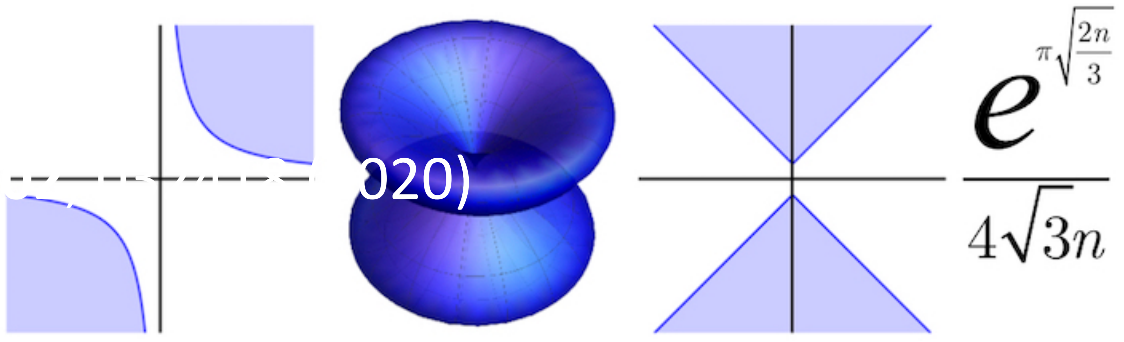
Spin 1 particle

$$S_x^2 = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}, \quad S_y^2 = \begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 1 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}, \quad S_z^2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

For spin-1 $[S_x^2, S_y^2] = [S_y^2, S_z^2] = [S_x^2, S_z^2] = 0.$

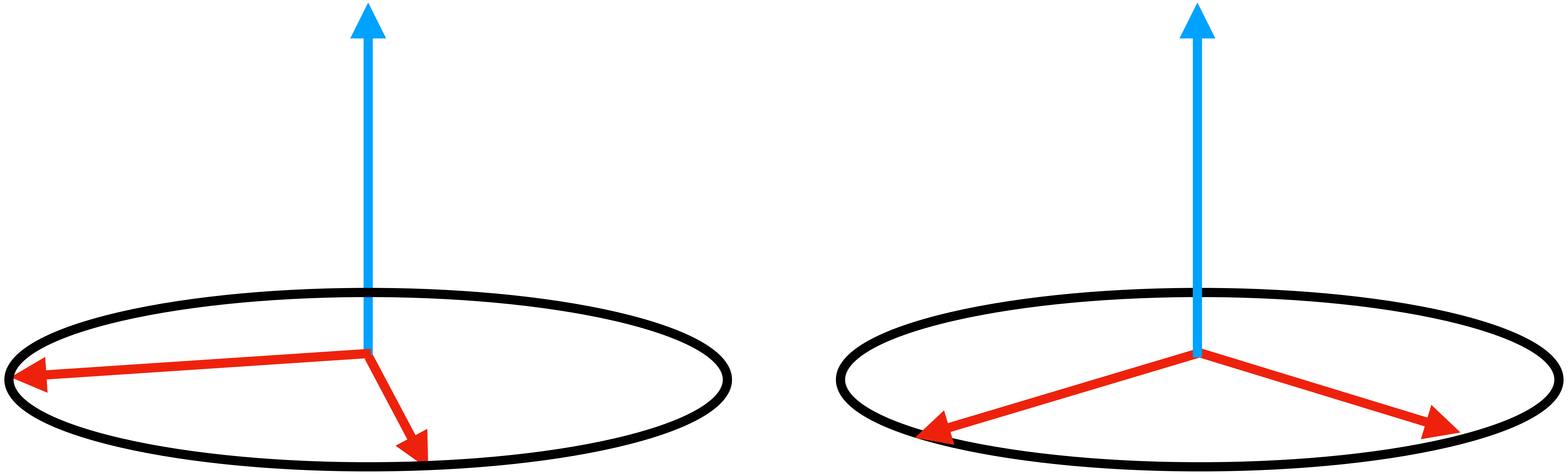
And we have a constraint that $S_x^2 + S_y^2 + S_z^2 = 2$

Assignments 0,1 to Sx, Sy, Sz must be 011, 101 or 110. Is this possible?



Example: Kochen-Specker paradox.

Assignments 0,1 to Sx, Sy, Sz must be 011, 101 or 110. Is this possible?



Context 1 Context 2

I need to decide for every context a consistent assignment 011: red red blue.

Example: Kochen-Specker paradox.

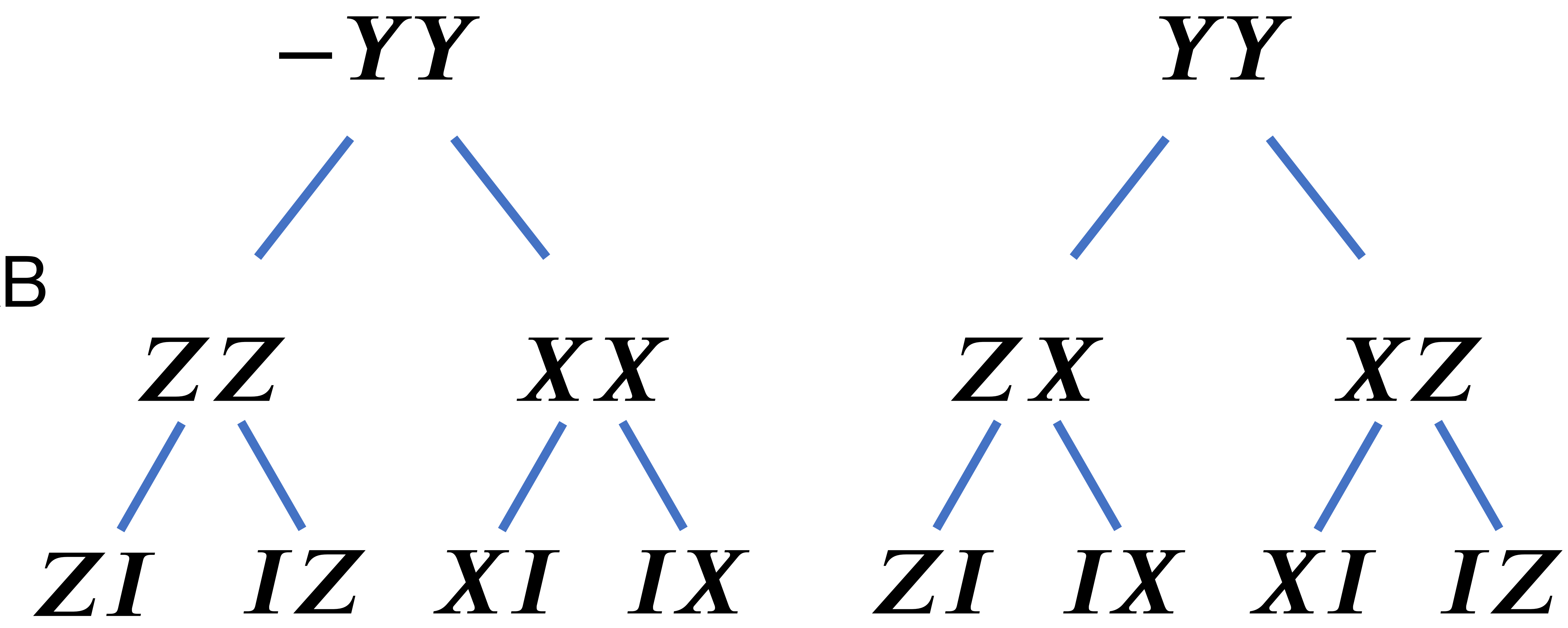
I need to decide for every context a consistent assignment 011: red red blue.

Example: Peres-Mermin Square

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

From A, B, [A,B]=0, can infer AB

Can infer AB from multiple contexts.

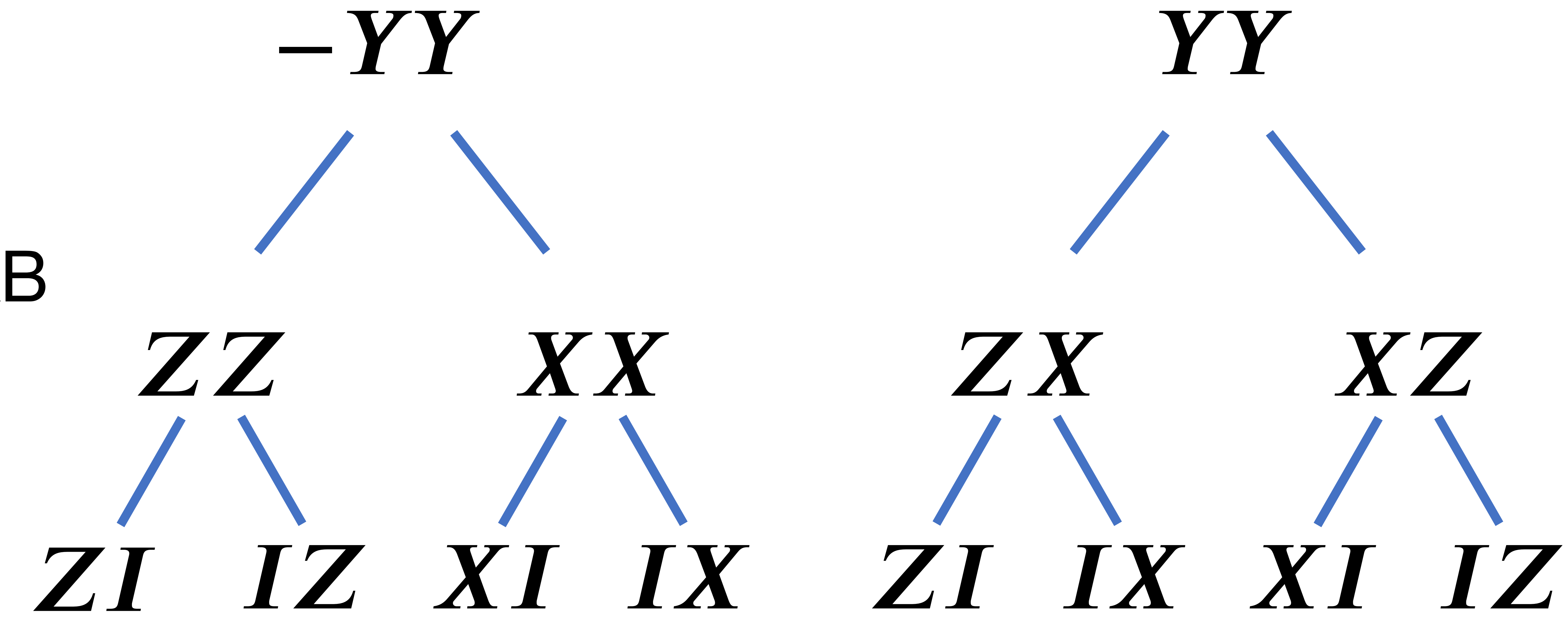


Given a joint value assignment to S we find that -YY and YY are assigned the **same value by two different contexts**

Contradiction: S is contextual

Obstacle: Contextuality

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



From A, B, [A,B]=0, can infer AB

Can infer AB from multiple contexts.

Peres: if f(A,B)=C for some f, then the assignments should also ensure f(a,b)=c

Contextuality: inferred values depend on *context* - grouping into commuting sets

Variational Quantum Eigensolver

Goal: Find ground state energy of: $H = \sum_{P_i \in S} \alpha_i P_i$

On a classical computer minimize:

$$E_0 \leq \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle = \sum_{P_i \in S} \alpha_i \langle \psi(\vec{\theta}) | P_i | \psi(\vec{\theta}) \rangle$$

- $|\psi(\vec{\theta})\rangle$ is prepared on quantum computer
- $\langle \psi(\vec{\theta}) | P_i | \psi(\vec{\theta}) \rangle$ is measured on quantum computer

Peruzzo, Alberto, et al. "A variational eigenvalue solver on a photonic quantum processor." *Nature communications* 5.1 (2014): 1-7.

Classical model?

Goal: Find **set S** such that we can create a **classical model**

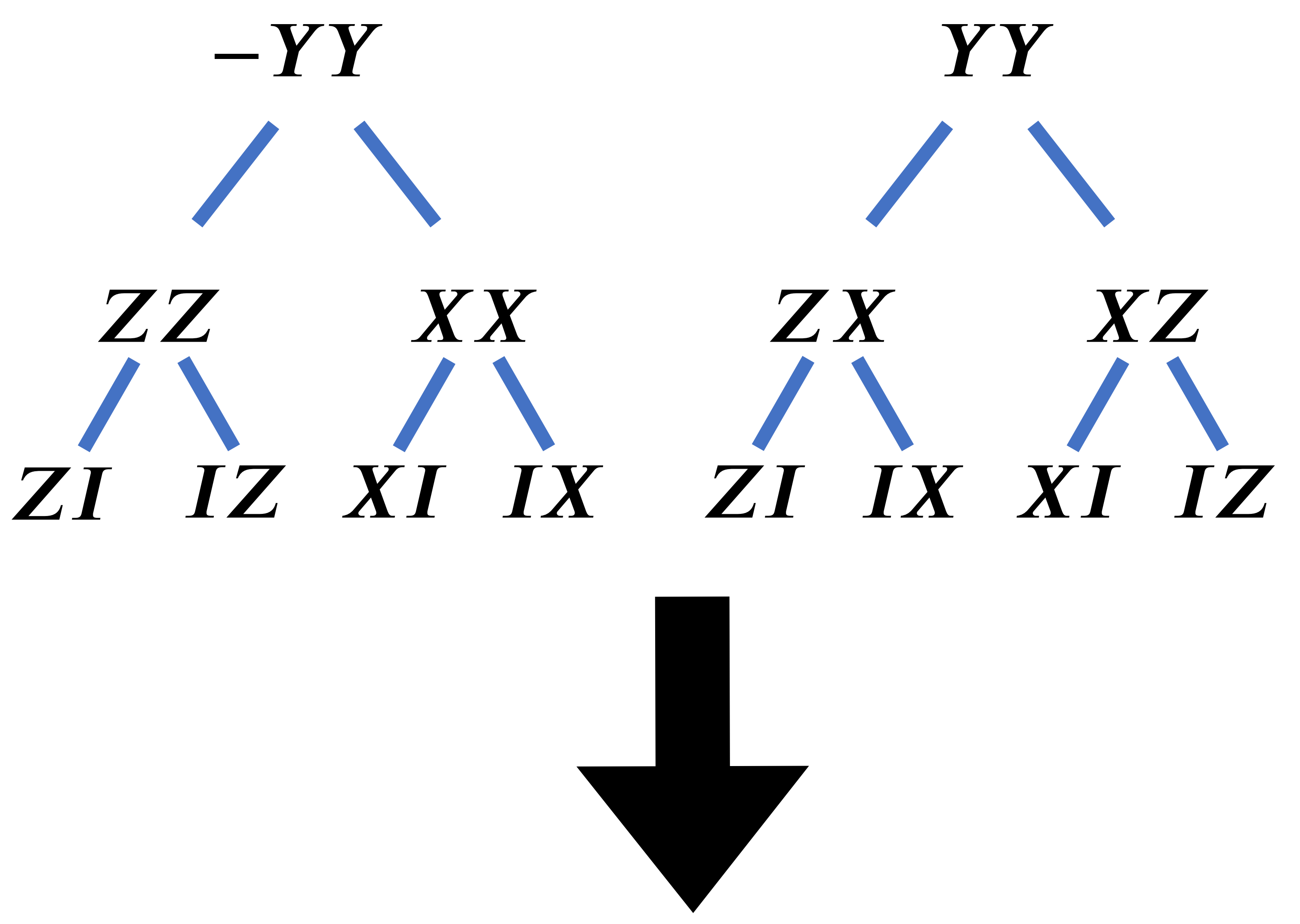
$$H = \sum_{P_i \in S} \alpha_i P_i$$

- Classically measurements reveal values of observables that existed before measurement (realism).
- Must be able to assign +/- values to observables in S without contradiction

When is a VQE experiment a test of fundamental quantum mechanics

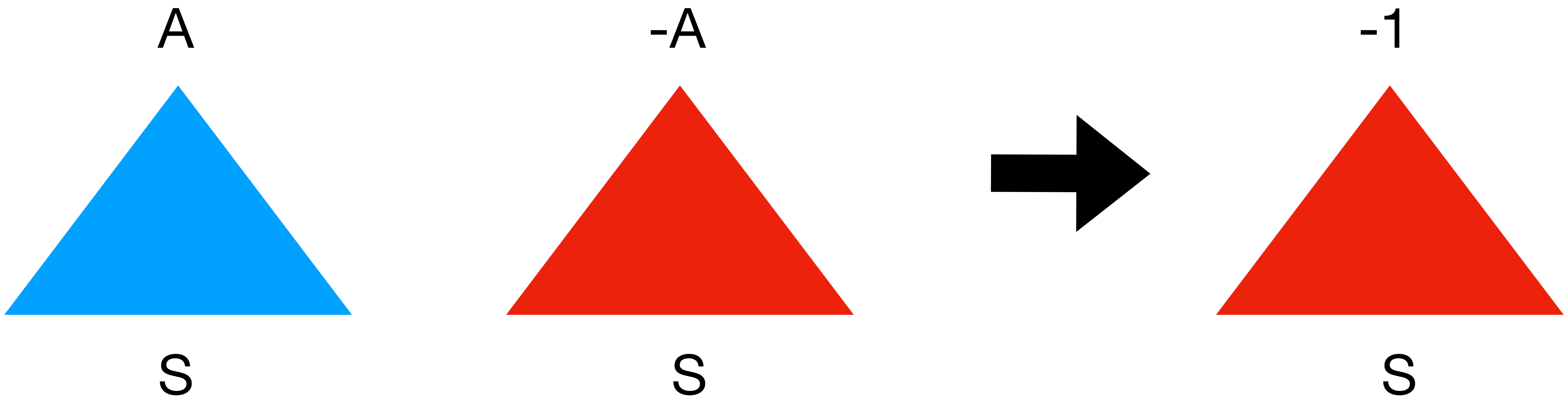
For any set of Pauli operators, when can we construct a Peres-Mermin type contradiction?

Generalizing Peres-Mermin



For a set of Pauli operators S its closure under inference $\bar{S}$ is the set of operators that can be formed from the Jordan Product:

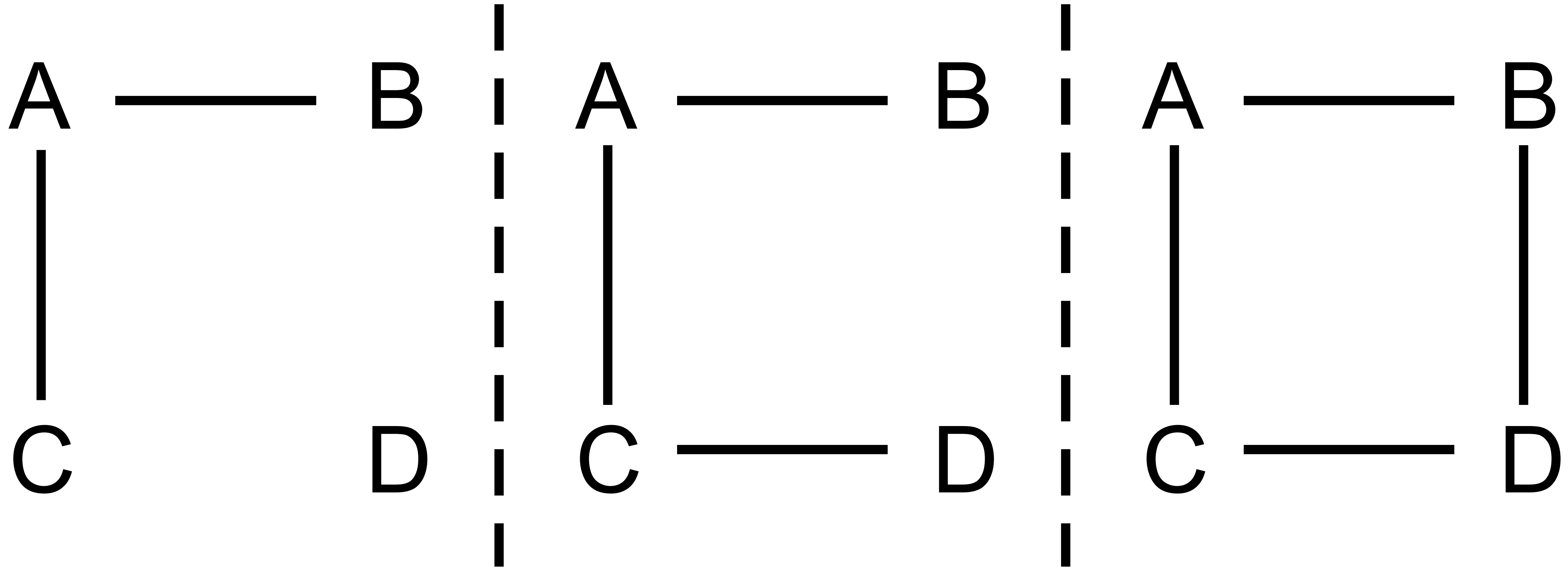
$$P \cdot Q = \frac{PQ + QP}{2}$$



Determining Trees

Generalizing Peres-Mermin

A set of four Pauli operators is contextual IFF it its compatibility graph is one of:



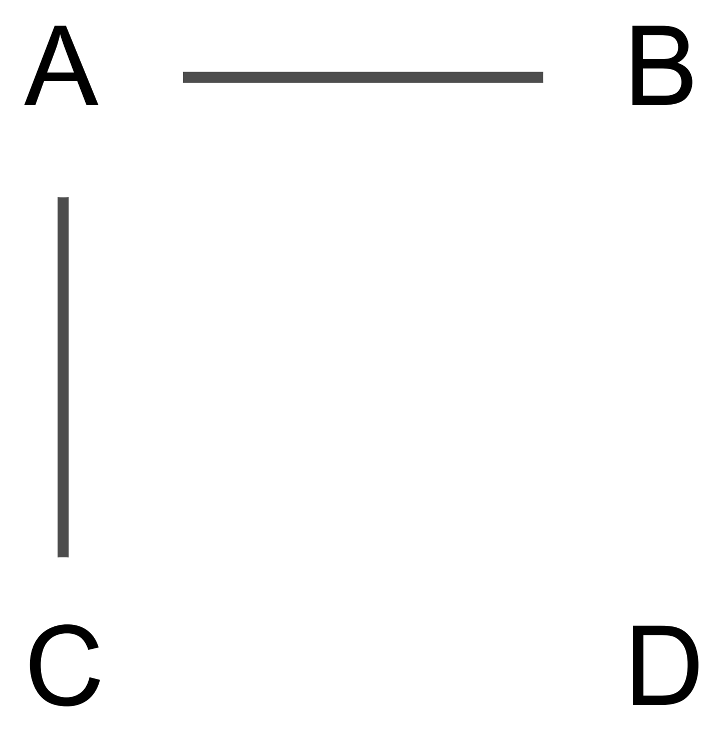
[A,B]=[A,C]=0

[A,B]=[A,C]=[C,D]=0

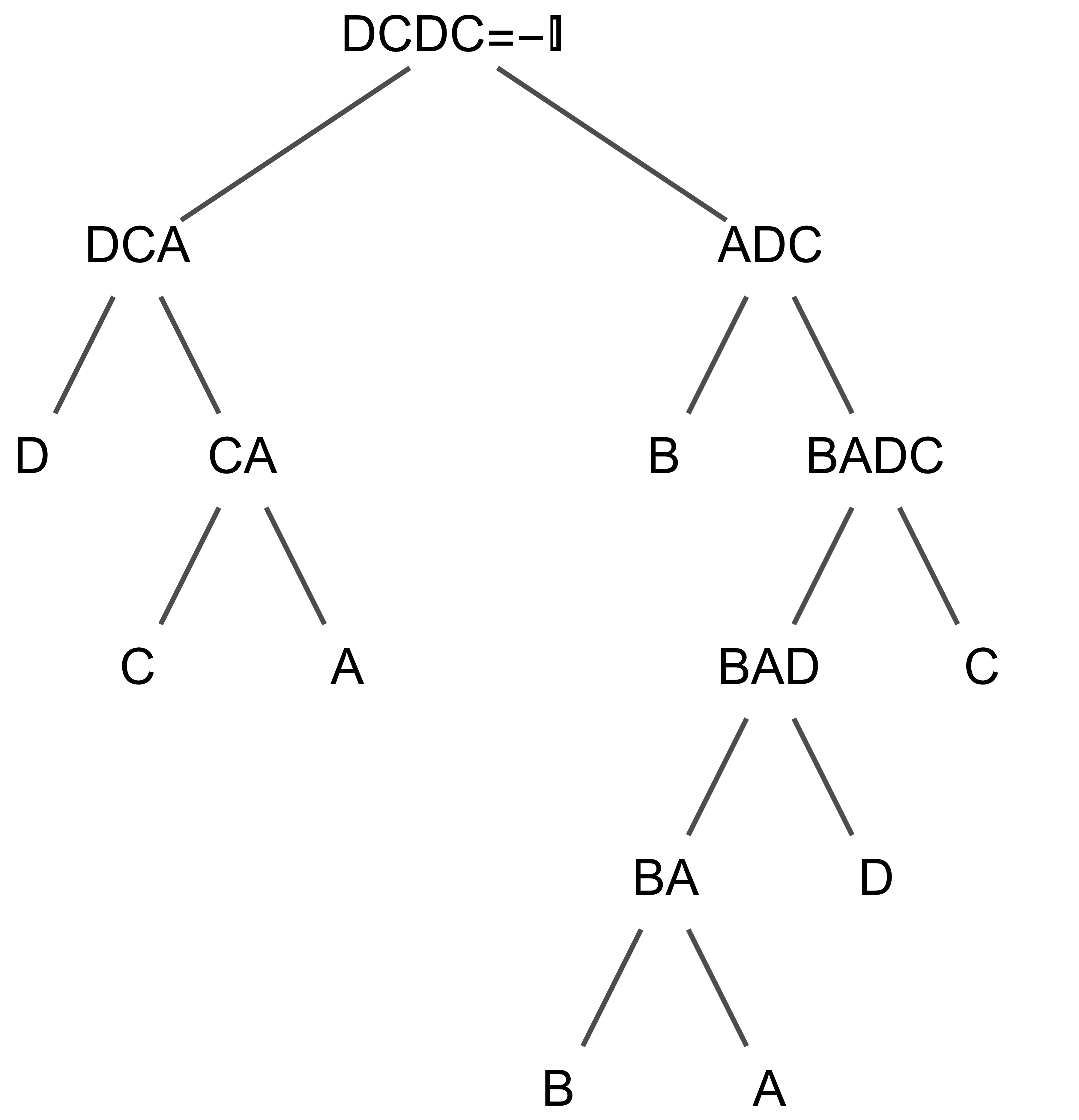
[A,B]=[A,C]=[C,D]=[B,D]=0

Fruit of forbidden trees I

Compatibility Graph



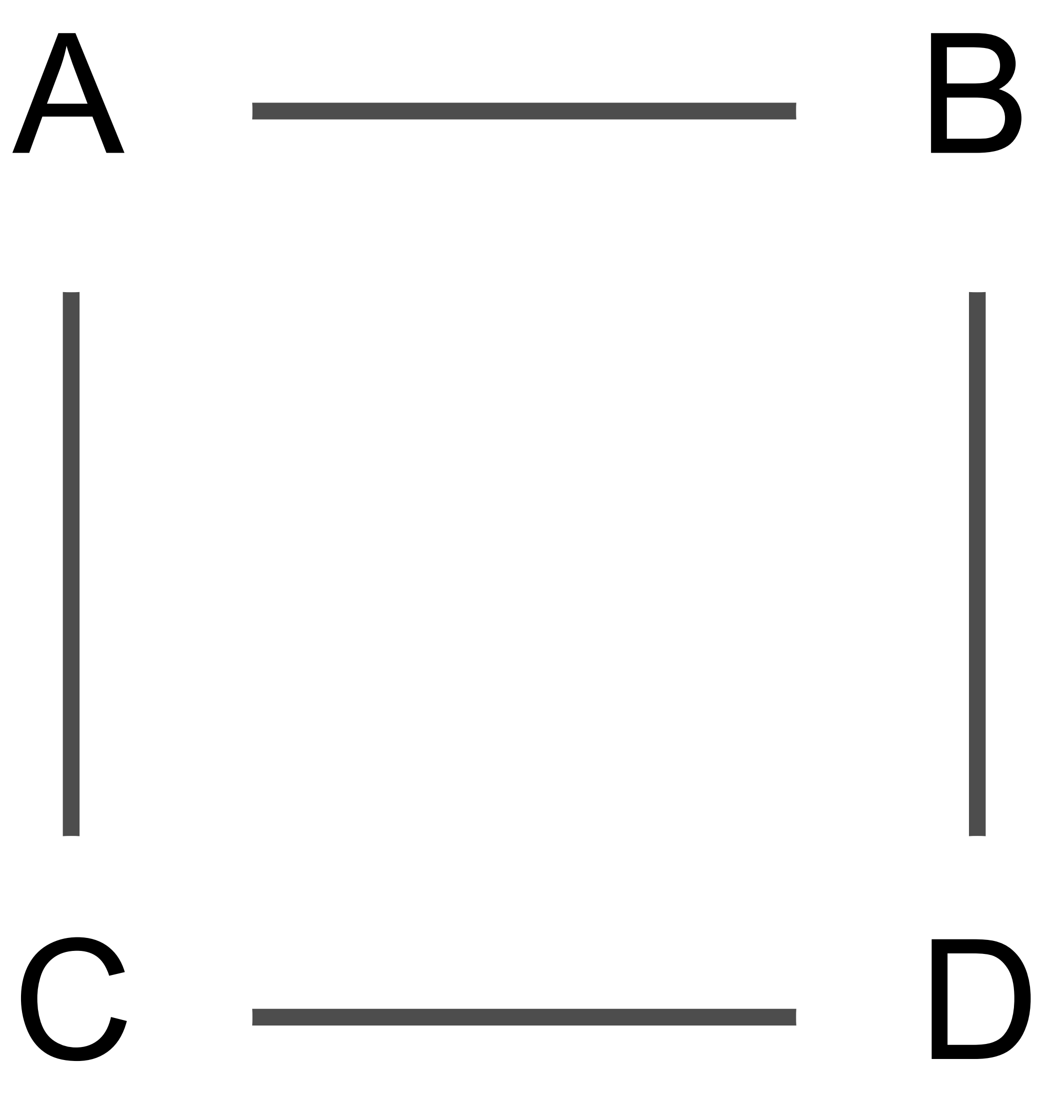
Determining Tree



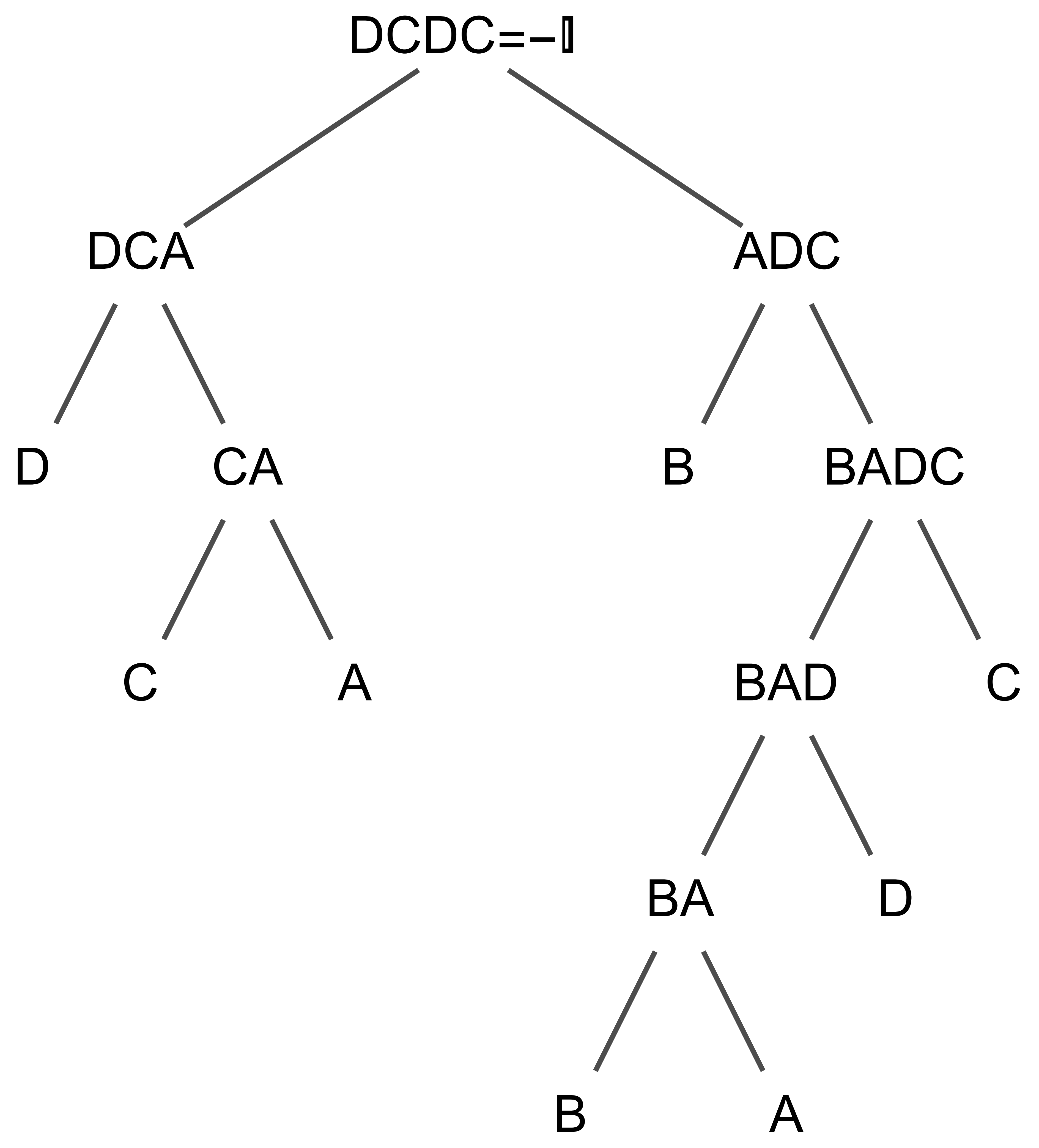
William M. Kirby and Peter J. Love
Phys. Rev. Lett. 123, 200501 (2019)

Fruit of forbidden trees II

Compatibility Graph



Determining Tree



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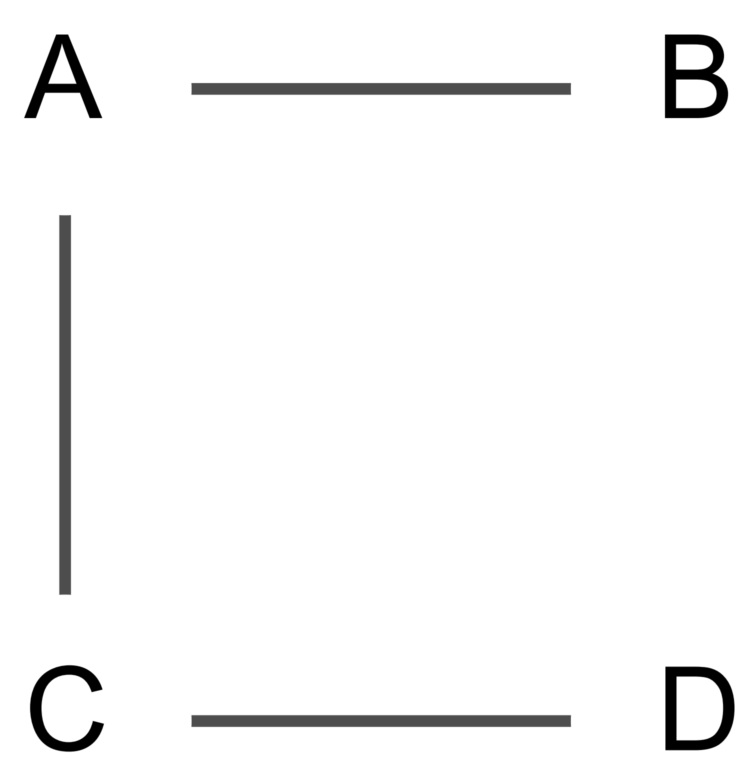
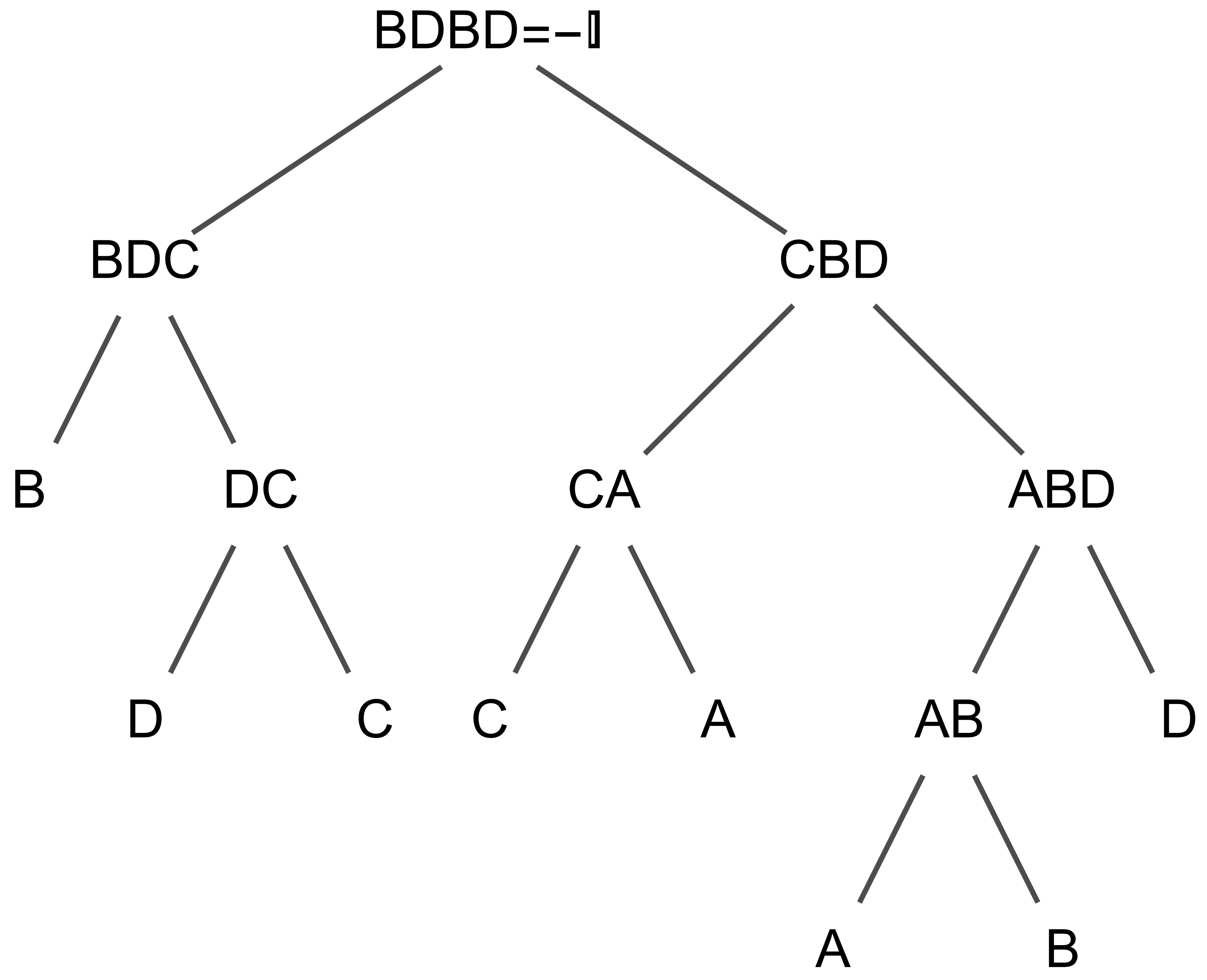
Fruit of forbidden trees III

Compatibility Graph

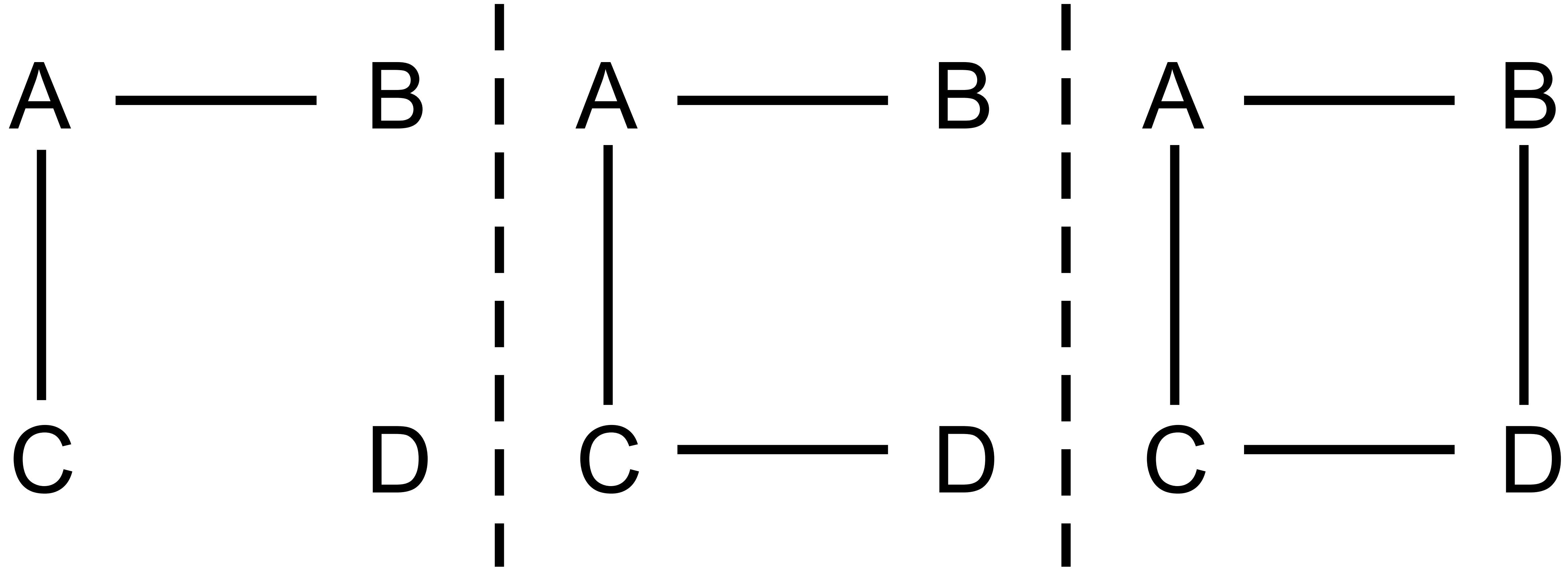


Determining Tree



Non-Contextual Pauli Sets

Raussendorf, Robert, Juani Bermejo-Vega, Emily Tyhurst, Cihan Okay, and Michael Zurel. "Phase-space-simulation method for quantum computation with magic states on qubits." *Physical Review A* 101, no. 1 (2020): 012350.



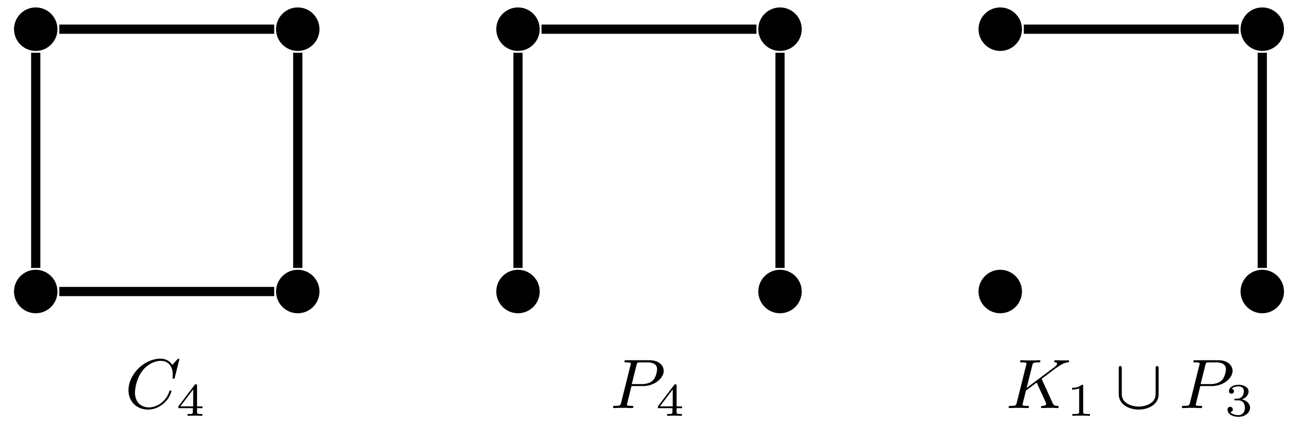


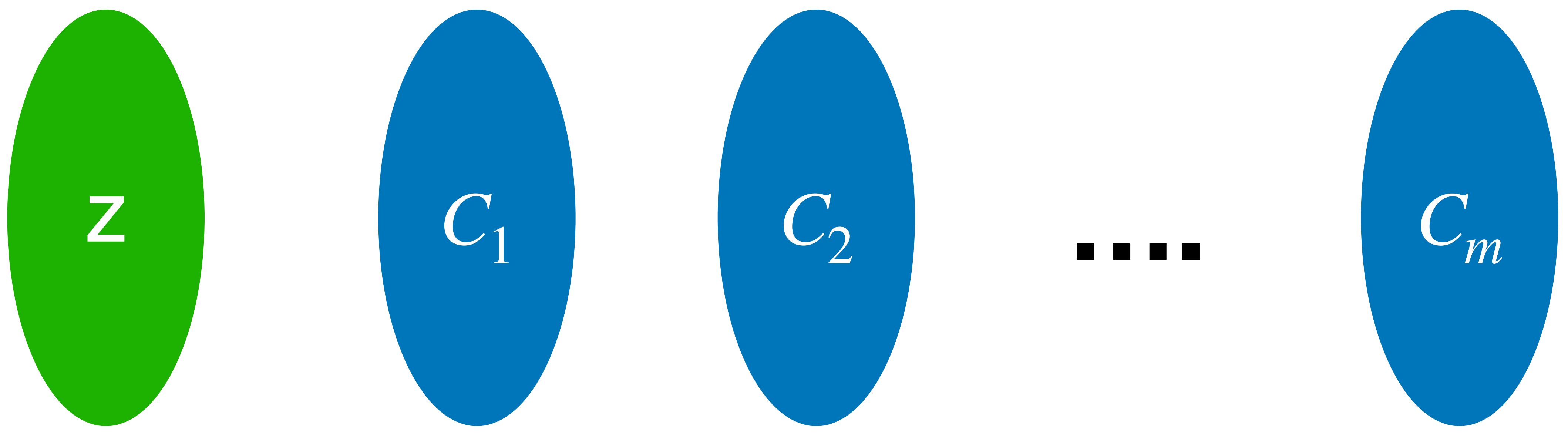
FIG. 4: Forbidden induced subgraphs of the commutativity graph, resulting from Mermin's square (also see [39]).

Theorem: A set of Pauli operators S is noncontextual iff the compatibility graph of the set with all globally commuting operators removed does not contain one of the above subgraphs. (independently discovered in)

Theorem: A set of Pauli operators S is noncontextual iff commutation is an equivalence relation on the set with all globally commuting operators removed.

William M. Kirby and Peter J. Love
Phys. Rev. Lett. 123, 200501 (2019)

Non-Contextual Pauli Sets



Theorem: A set of Pauli operators S is noncontextual iff it has the structure:

$$S = Z \cup T = Z \cup C_1 \cup C_2 \cup \ldots \cup C_m \qquad m \leq 2n + 1$$

T is defined by the fact that commutation is an equivalence relation on T

C's are completely commuting cliques. Operators from different cliques anti commute.

A Noncontextual Pauli Hamiltonian is a Pauli Hamiltonian with terms drawn from a noncontextual set.

William M. Kirby and Peter J. Love
Phys. Rev. Lett. 123, 200501 (2019)

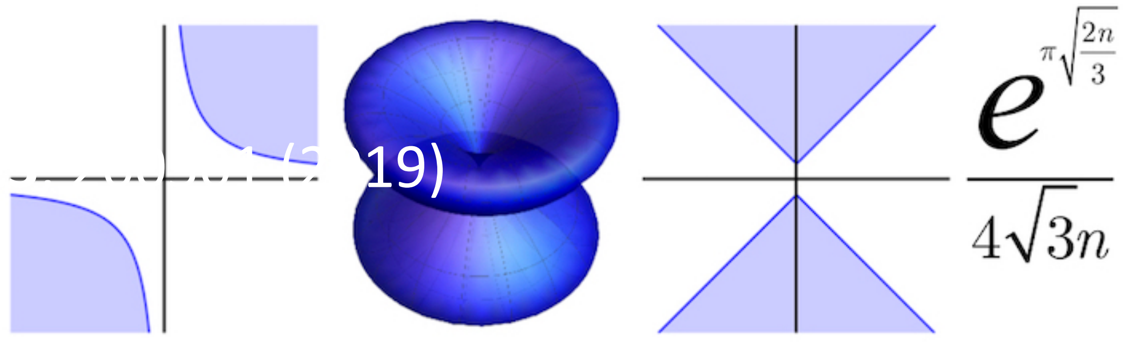
Are VQE experiments to date (before 2019) exploring Quantum problems?

Definition: Pauli Hamiltonian H is noncontextual iff its set of Pauli terms S is noncontextual

Citation:	System:	Contextual?
Dumitrescu *et al.* [22]	Deuteron	No
Kandala *et al.* [17]	H_2	No
O'Malley *et al.* [13]	H_2	No
Hempel *et al.* [18]	H_2 (BK)	No
Hempel *et al.* [18]	H_2 (JW)	No
Colless *et al.* [19]	H_2	No
Kokail *et al.* [23]	Schwinger Model	Yes
Nam *et al.* [20]	H_2O	Yes
Hempel *et al.* [18]	LiH	Yes
Peruzzo *et al.* [11]	HeH^+	Yes
Kandala *et al.* [17]	BeH	Yes
Kandala *et al.* [17,21]	LiH	Yes

Updated from
William M. Kirby and Peter J. Love Phys. Rev. Lett. 123, 200501 (2019)

Test is implemented in OpenFermion



Can Classical Noncontextual Model beat VQE?

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, 0.0016 Ha. Experimental errors preceded by $\sim$ were estimated from figures.

Error noncon

Error VQE

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}	
Peruzzo *et al.*, 2014 [2]	HeH^+	2	9	5	3	0.21	4.1	4.1	✓
Hempel *et al.*, 2018 [11]	LiH	3	13	9	4	0.56	0.56	$\sim$80	✓
Kandala *et al.*, 2017 [10]	LiH	4	99	23	5	4.2	9.3	$\sim$30	✓
Kandala *et al.*, 2017 [10]	BeH_2	6	164	42	7	156	266	$\sim$90	✗

can we do better?

William M. Kirby and Peter J. Love, Phys. Rev. A 102, 032418 (2020)

The Contextual Subspace Approach

$$H = H_{noncon} + H_{con}$$

Solve on classical computer

Solve on quantum computer

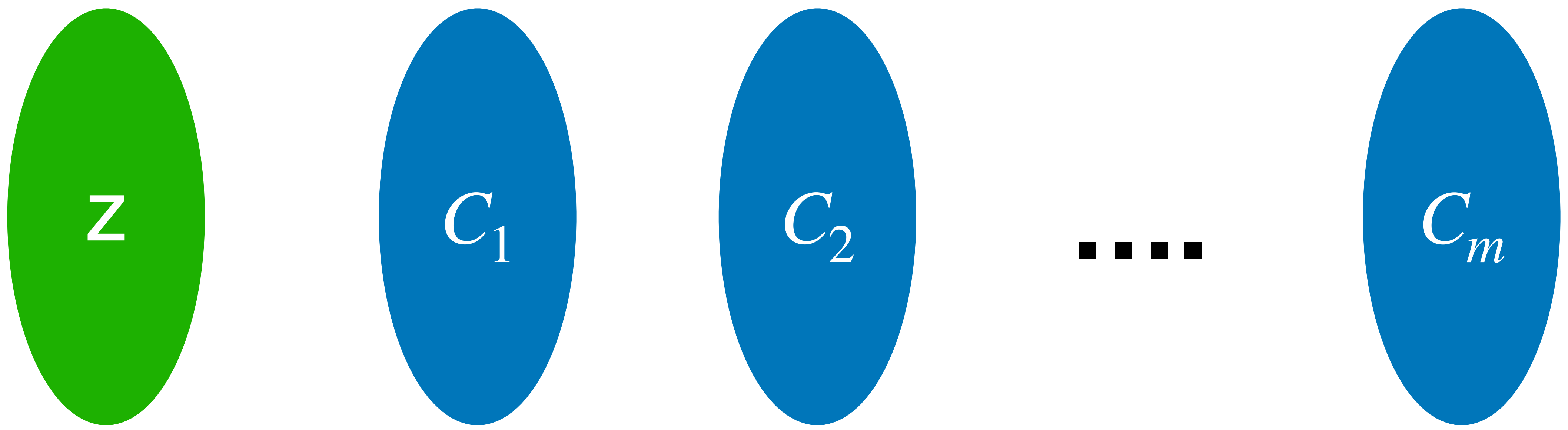
$$UHU^{\dagger} \neq VH_{noncon}V^{\dagger} + WH_{con}W^{\dagger}$$

Need to **define a VQE algorithm for** H_{con} in <u>**subspace**</u> consistent with ground state of H_{noncon}

Subspace methods

- Qubit Tapering
  - Exploits physical symmetries (spin parity, point groups…)
  - Reduction by <u>one qubit for each symmetry</u>
- Contextual Subspace
  - $H = H_{\text{noncon}} + H_{\text{context}}$
  - Imposing noncontextual ‘symmetries’ on H_{context} causes systematic error, but gives a smaller (higher precision) VQE problem.
  - Can increase size of H_{Context} to reduce errors.

Non-Contextual Pauli Sets



For n qubits there are at most 2n+1 cliques.

Theorem: A set of Pauli operators S is noncontextual iff it has the structure:

$$S = Z \cup T = Z \cup C_1 \cup C_2 \cup \ldots \cup C_m \qquad m \leq 2n + 1$$

T is defined by the fact that commutation is an equivalence relation on T

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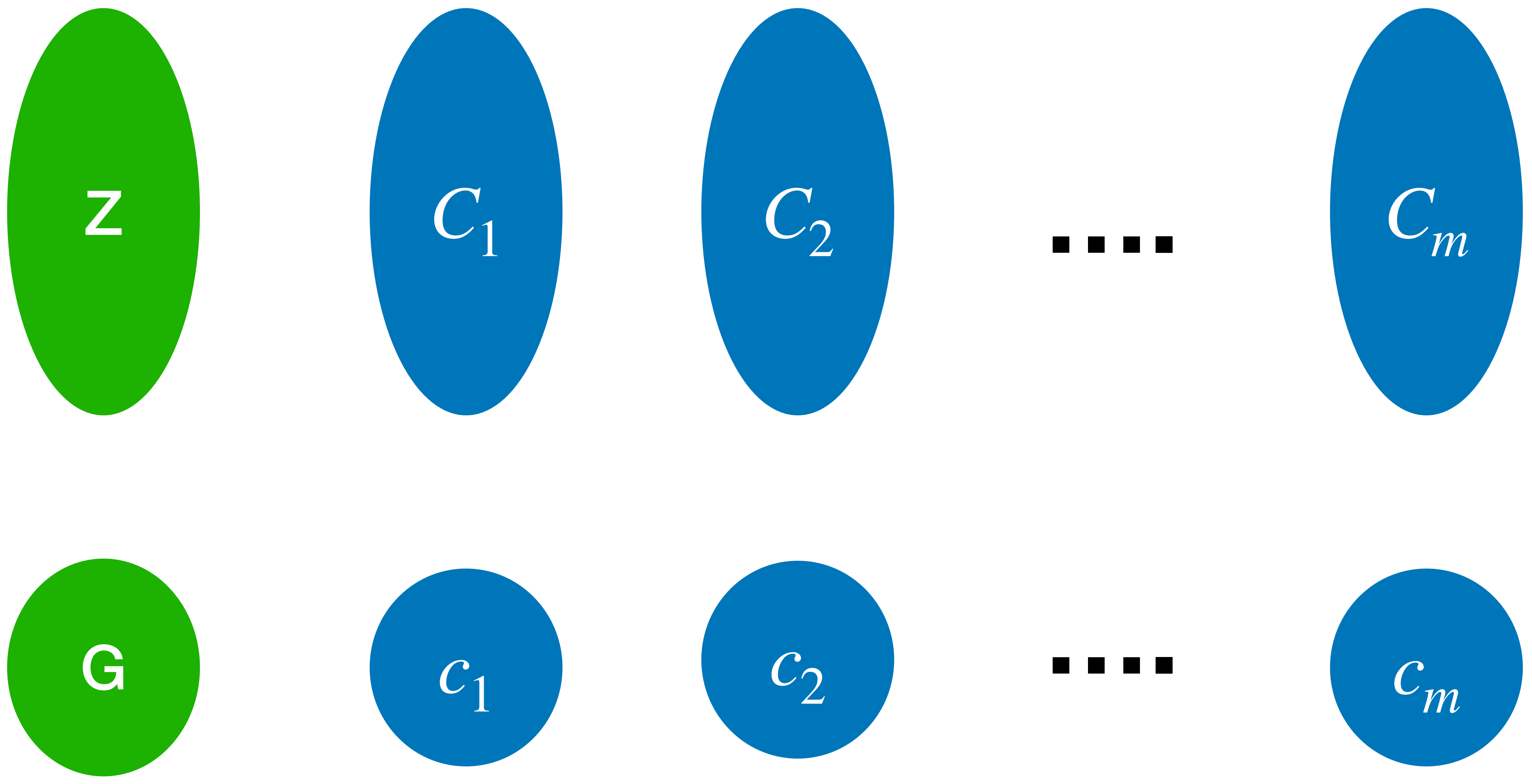
Phys. Rev. Lett. 123, 200501 (2019)

Non contextual Hamiltonians



Clique representatives

$$H = \sum_{P_j \in Z} a_j P_j + \sum_k c_k \sum_{P_j \in Z} b_{jk} P_j$$

Stabilizer Hamiltonian

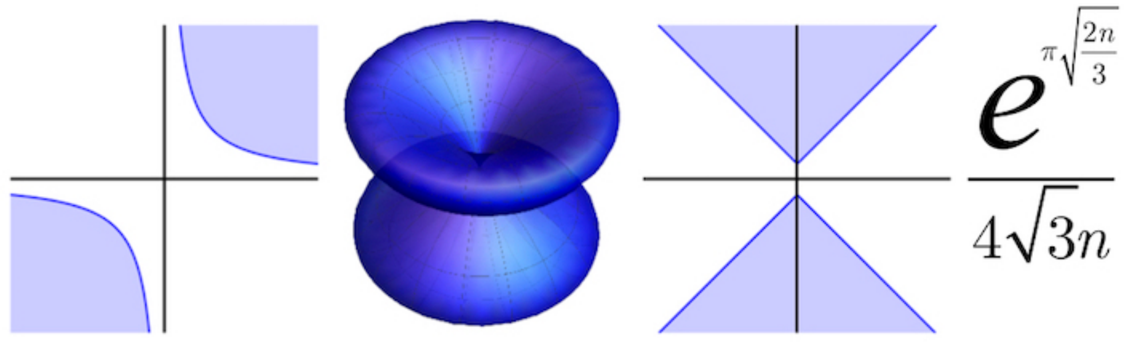
Clique elements

Eigenvalues of stabilizer generators $\vec{\nu}$ fix symmetry sector:

$$H^{\vec{\nu}} = E_{\vec{\nu}} 1 + \sum_k \gamma_k^{\vec{\nu}} c_k \qquad \text{spectrum: } E_{\vec{\nu}} = \lambda_{\vec{\nu}} \pm |\gamma^{\vec{\nu}}|$$

Rotate anticommuting c_k to a single Pauli by non-clifford unitary R.

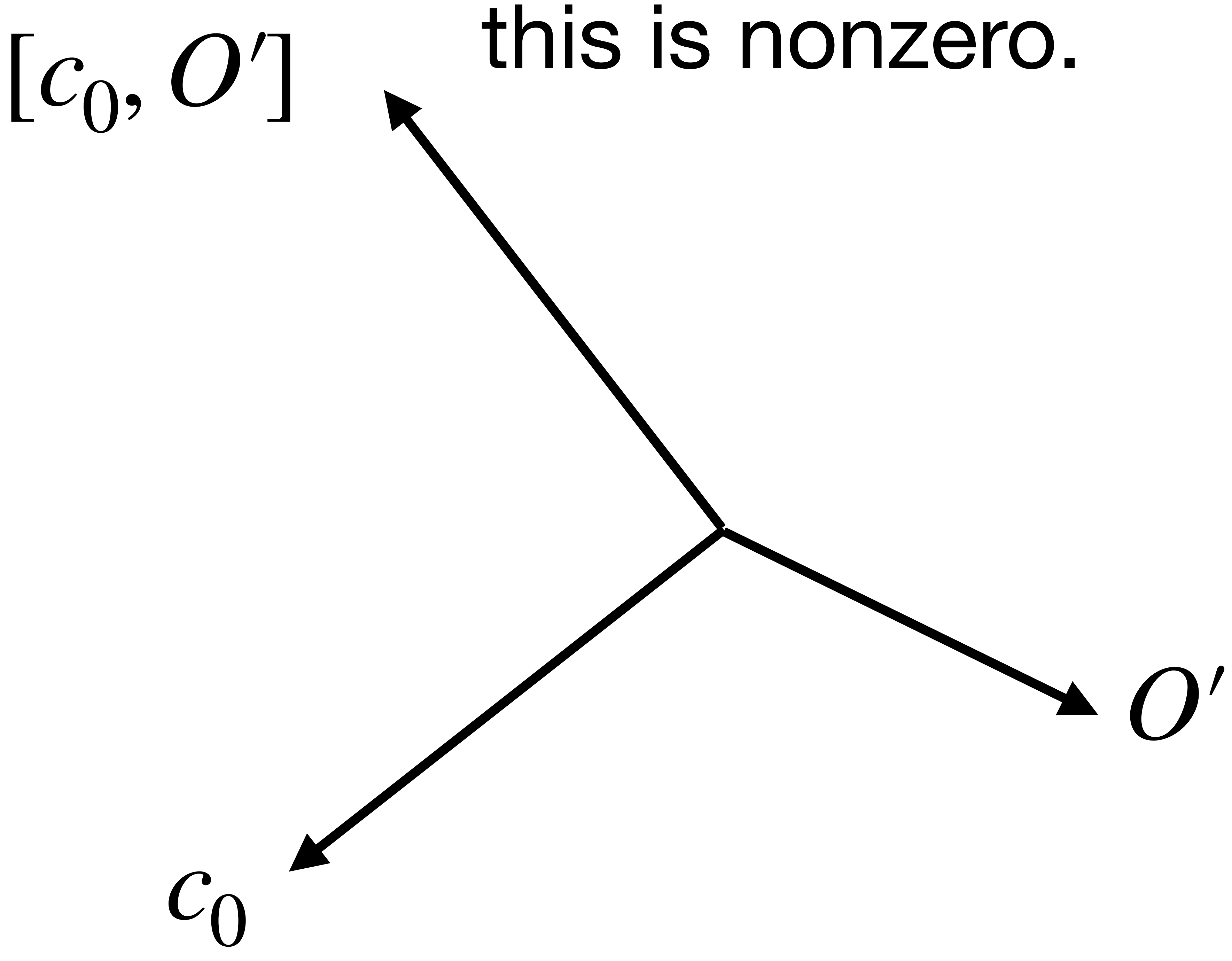
Noncontextual Pauli Hamiltonians, A. Ralli, T. Weaving, P. J. Love, Phys. A: Math. Theor. 58 335301, (2025)



Eigenspaces

$$H^{\vec{\nu}} = E_{\vec{\nu}} 1 + \sum_k \gamma_k^{\vec{\nu}} c_k = E_{\vec{\nu}} 1 + |\gamma^\nu| \left(a c_0 + O' \right)$$

Note c_0 and O' anti-commute so this is nonzero.



Rotate this to:

$$R^\dagger H^{\vec{\nu}} R = E_{\vec{\nu}} 1 + |\gamma^\nu| a' c_0$$

Rotation generated by:

$$[c_0, \sum_{k>1} \bar{\gamma}_k^{\vec{\nu}} c_k] = 2 \sum_{k>1} \bar{\gamma}_k^{\vec{\nu}} c_0 c_k$$

a linear combination of m-1 anti-commuting Paulis

Eigenspaces

Generically a non-clifford rotation R generates magic (rapidly!)

But R has the form:

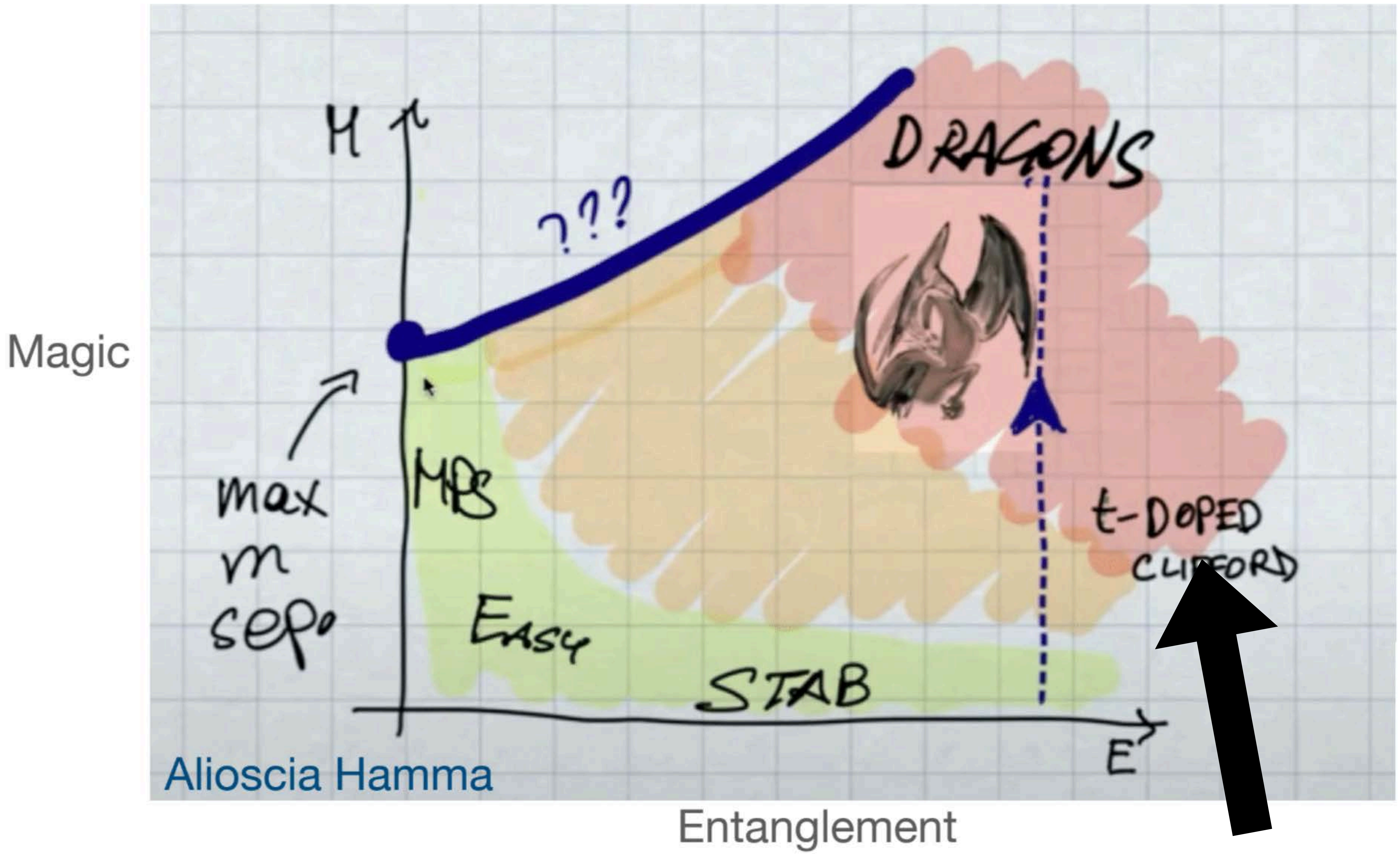
$$R = \cos\theta \mathbb{1} + i\sin\theta \sum_{k>1}^{m} \alpha_k c_k$$

This means R acting on a stabilizer state generates a state with stabilizer rank m.

So each (degenerate) eigenspace of a noncontextual Hamiltonian contains a state of at most linear stabilizer rank.

This means only at most short-range magic, as such states can be generated by log depth circuits.

Eigenspaces



We are here!

R has the form:

$$R = \cos\theta \mathbb{1} + i \sin\theta \sum_{k>1}^{m} \alpha_k c_k$$

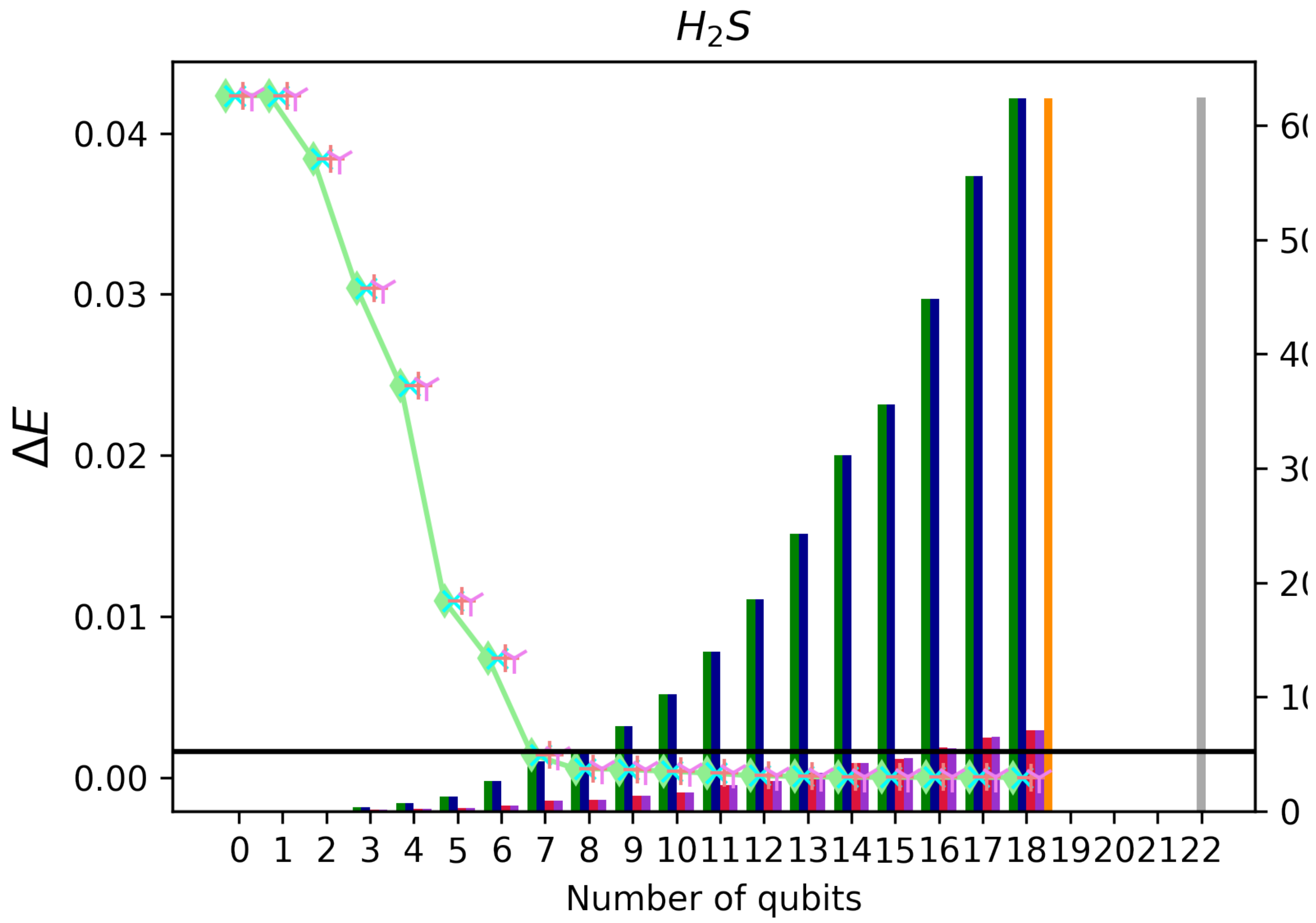
where $m \leq 2n + 1$

R: stabilizers-> states with linear stabilizer rank.

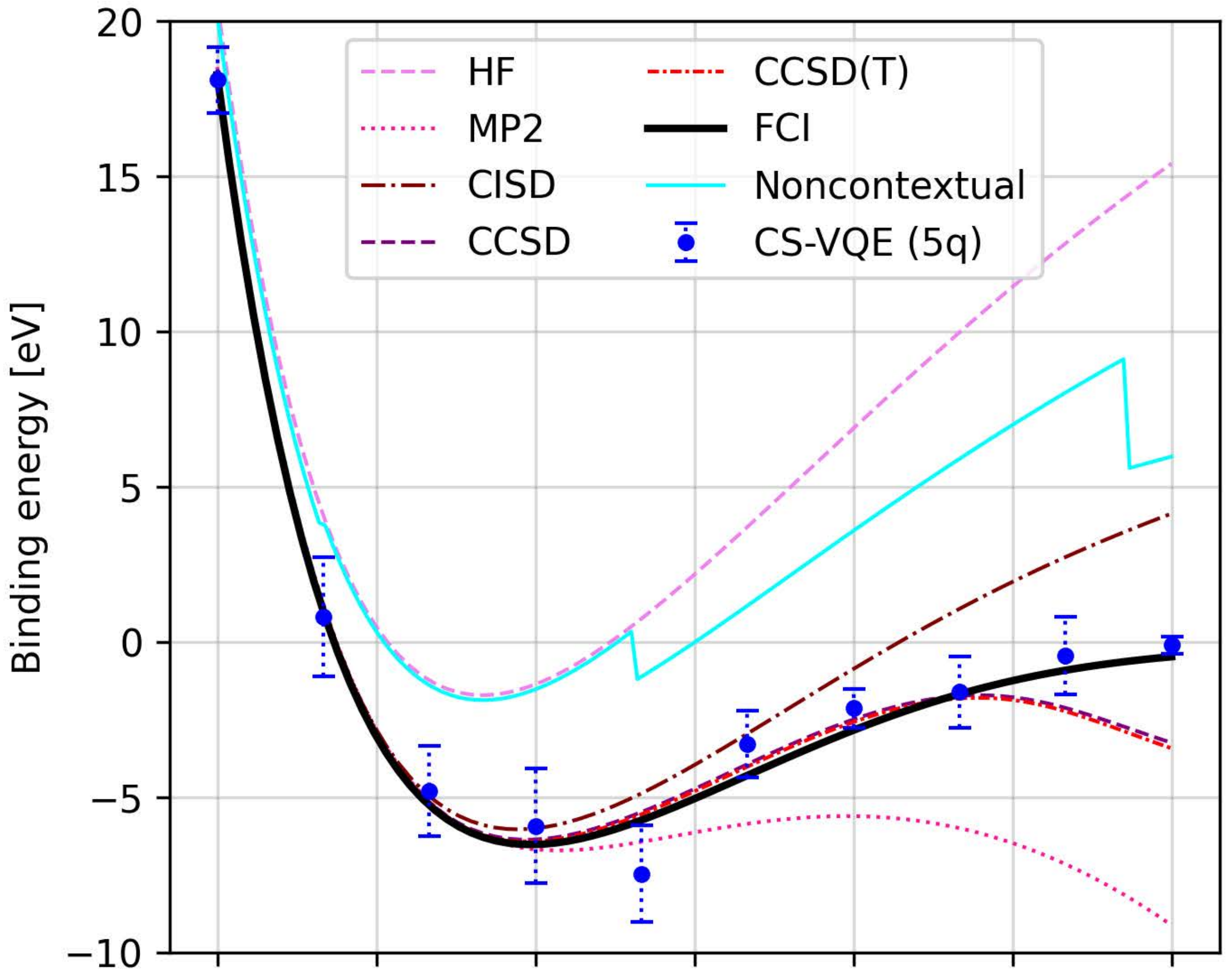
Also called local magic

Leone, L., Oliviero, S.F. and Hamma, A., 2022. Stabilizer rényi entropy. Physical Review Letters, 128(5), p.050402.

Noncontextual Chemistry: Examples



H_2S 22 -> 7 qubits



N_2 15->11 qubit

SpacePulse: Combining Parameterized Pulses and Contextual Subspace for More Practical VQE

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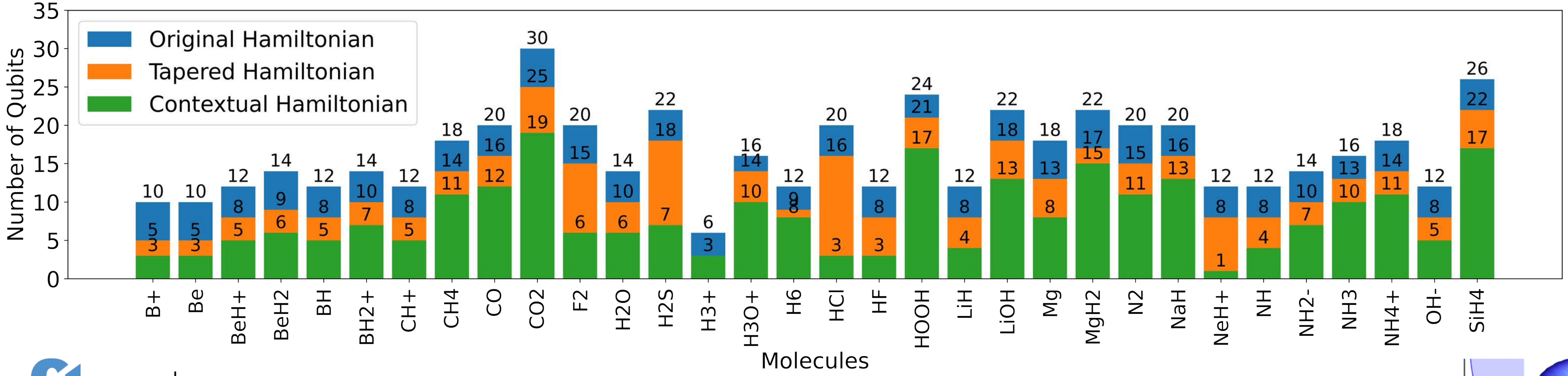
Zhixin Song* Georgia Institute of Technology Atlanta, GA, USA
Jinglei Cheng* Purdue University West Lafayette, IN, USA
Hang Ren* University of California, Berkeley Berkeley, CA, USA
Tianyi Hao* University of Wisconsin-Madison Madison, WI, USA
Rui Yang* Peking University Beijing, China
Yiyu Shi University of Notre Dame Notre Dame, IN, USA
Tongyang Li Peking University Beijing, China



Measuring Magic

Non-stabilizerness and contextuality close, but not exactly the same for qubits.

Useful to have a quantitative measure of nonstabilizerness/Magic.

We can measure the amount of magic in a state using the **stabilizer Rényi entropy (SRE)**

$$M_2(\psi) = -\log_2\left(\sum_{P\in\{I,X,Y,Z\}^{\otimes n}} \frac{\left|\langle\psi|P|\psi\rangle\right|^4}{2^n}\right)$$

L. Leone *et al.*, “Stabilizer Rényi entropy,” Phys. Rev. Lett. **128**, 050402 (2022)
T. Haug and L. Piroli, “Stabilizer entropies and nonstabilizerness monotones,” Quantum **7**, 1092 (2023)

Stabilizer Rényi Entropy

$$M_2(\psi) = -\ln\left(\sum_{P\in\{I,X,Y,Z\}^{\otimes n}} \frac{\left|\langle\psi|P|\psi\rangle\right|^4}{2^n}\right)$$

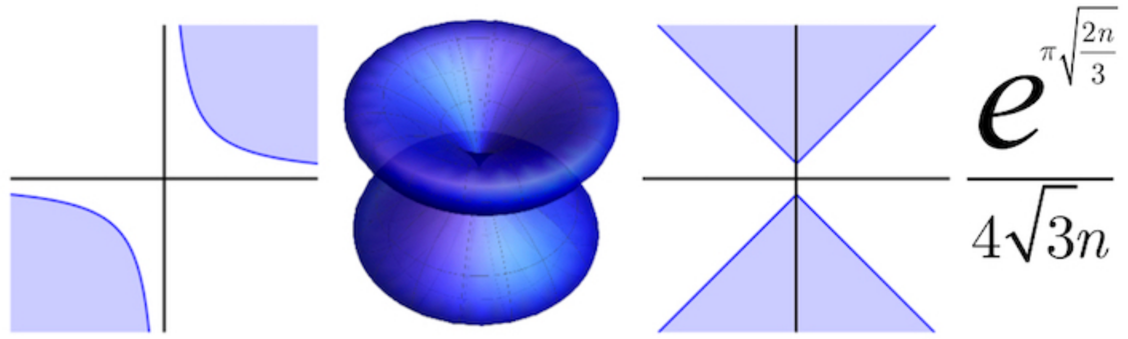
$|\mathrm{STAB}\rangle$ ⟷ $|\mathrm{HAAR}\rangle$

$M_2 = 0$ $\qquad$ $M_2 \approx n - 2$

$$p(P_i) = \frac{|\langle\psi|P_i|\psi\rangle|^2}{2^n} \qquad 0 \le p(P_i) \le 1, \quad \sum_i p(P_i) = 1$$

$$M_2(\psi) = -\log_2 \sum_i p_i^2$$

L. Leone *et al.*, “Stabilizer Rényi entropy,” Phys. Rev. Lett. **128**, 050402 (2022)
L. Bittel and L. Leone, “Operational interpretation of the Stabilizer Entropy”, Quantum (in press)
S. F. E. Oliveiro *et al*., “Measuring magic on a quantum processor”, npj Quantum Information **8** 148 (2022)

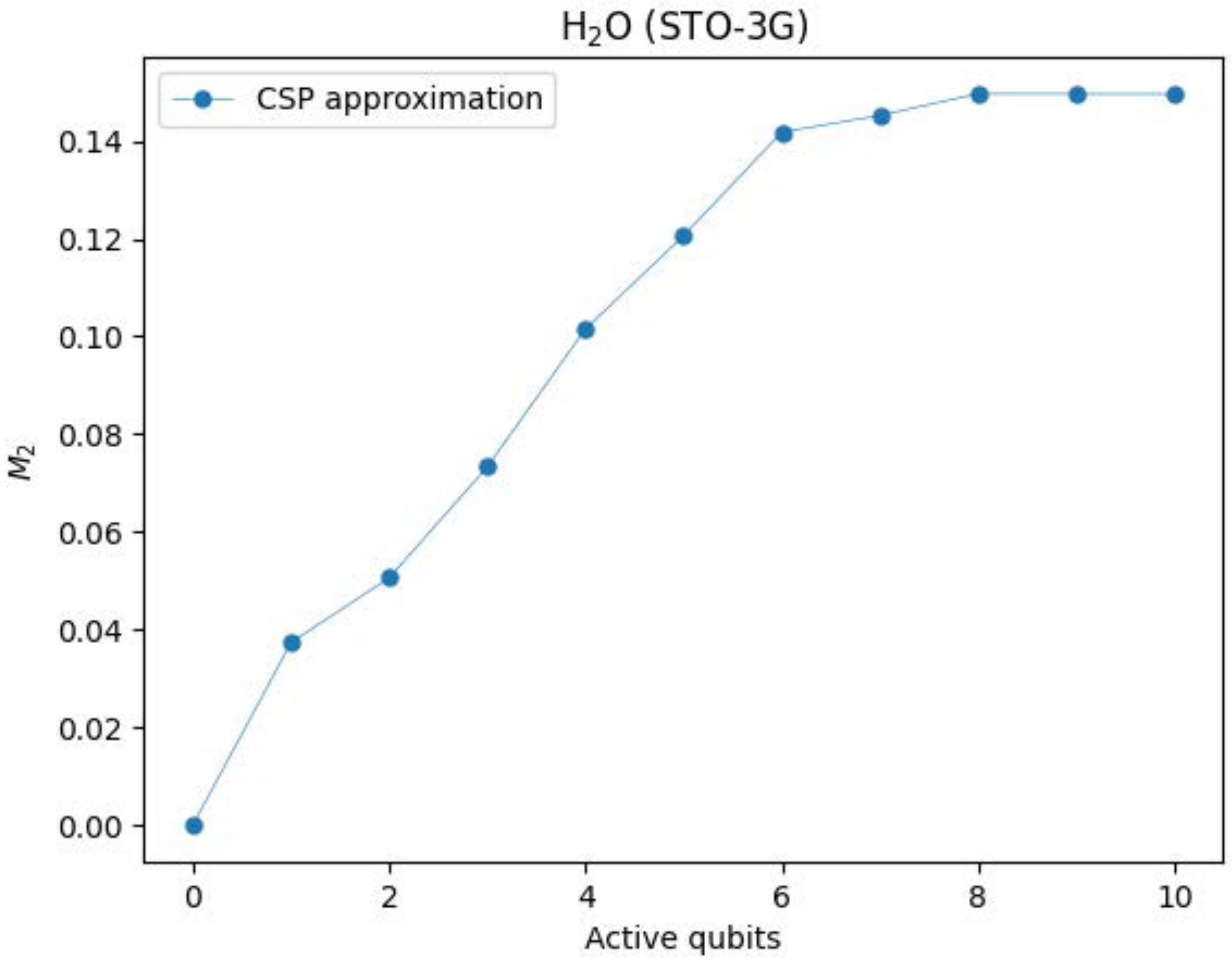


Magic in contextual subspace projection

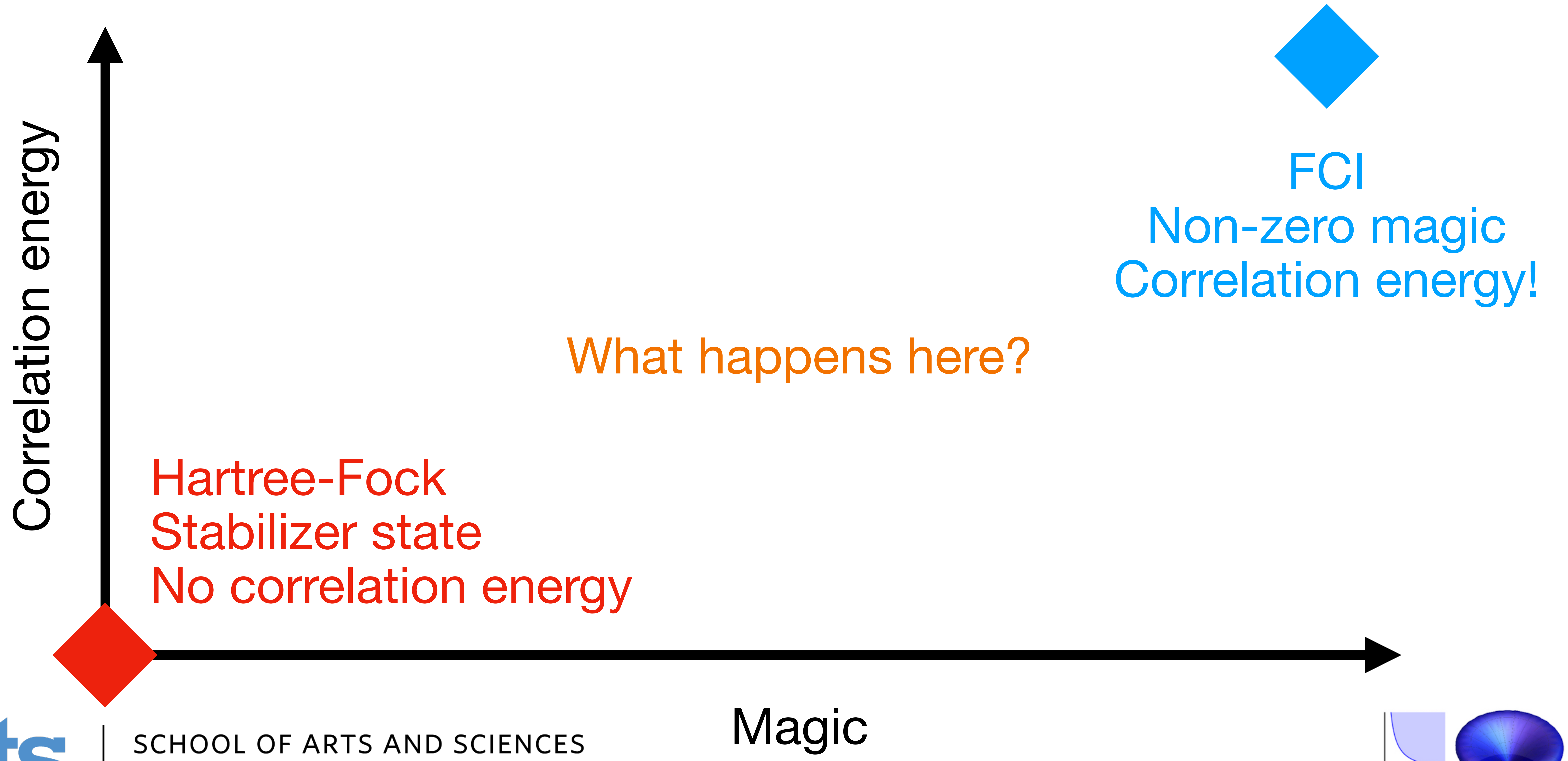
Use stabilizer Rényi entropy to quantify how the ground state magic changes through contextual subspace projection

$$M_2(\psi) = -\ln\left(\sum_{P\in\{I,X,Y,Z\}^{\otimes n}} \frac{\left|\langle\psi|P|\psi\rangle\right|^4}{2^n}\right)$$

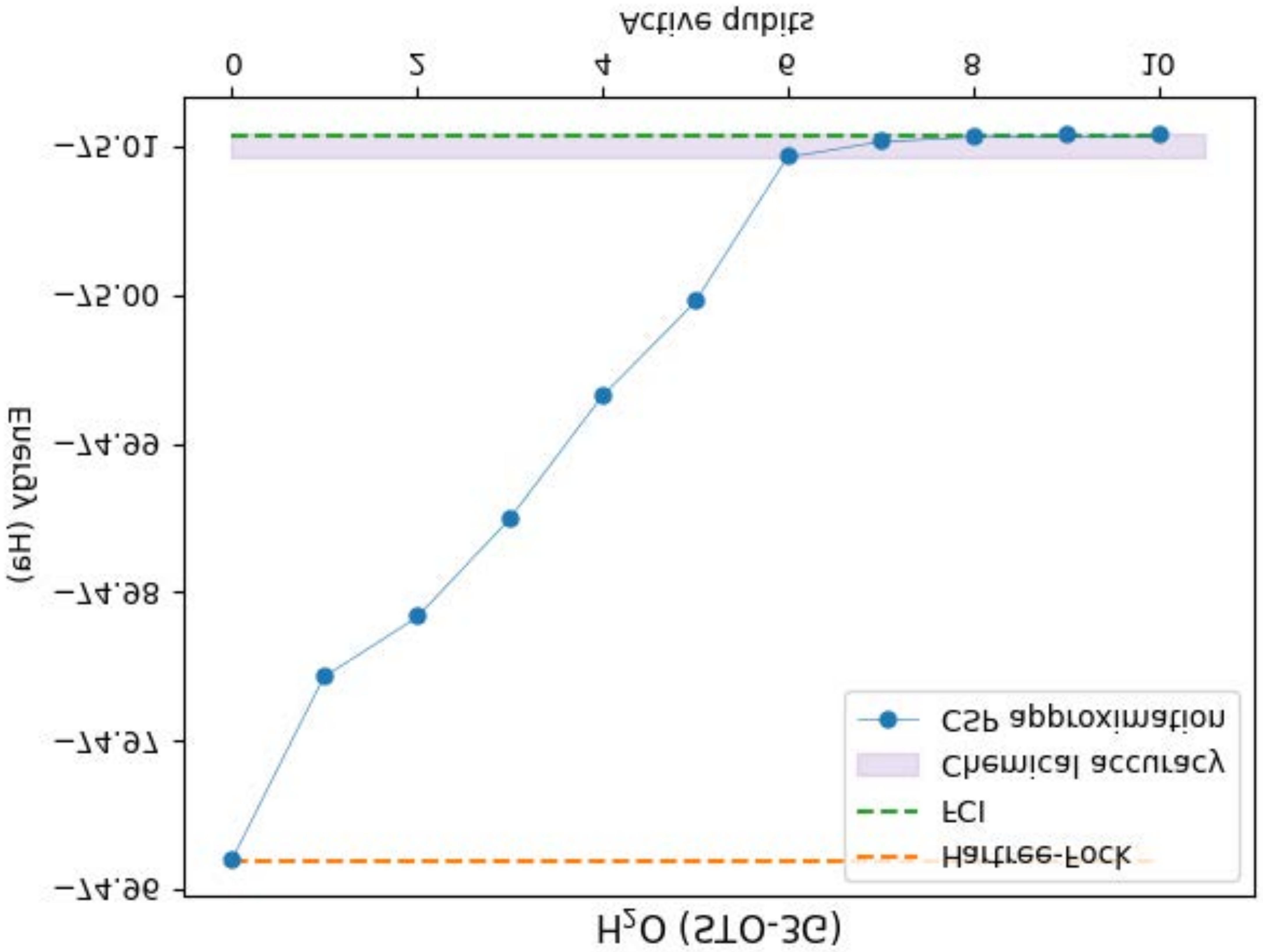
Find numerical evidence that SRE **monotonically increases** as more qubits are added to the contextual subspace

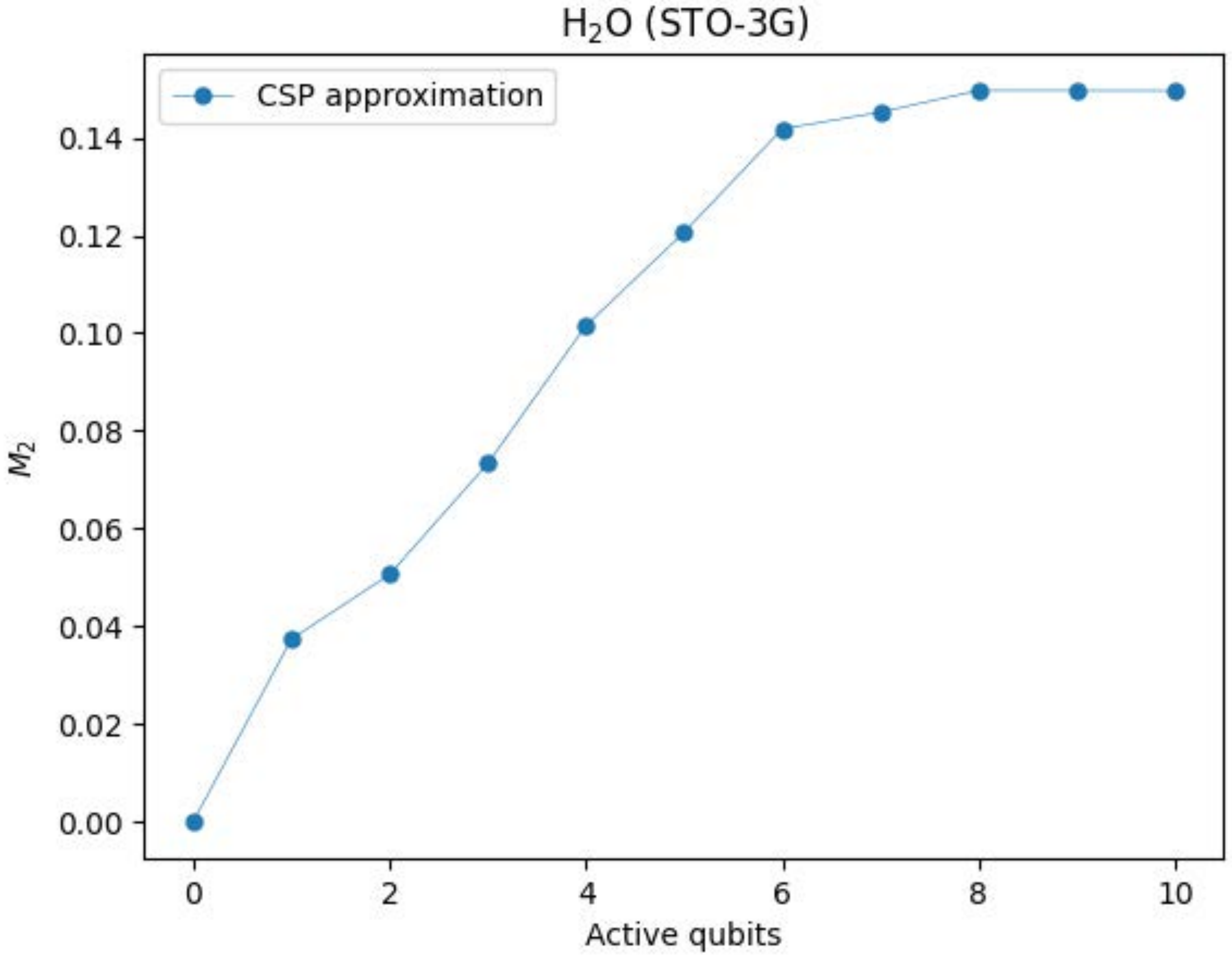


Magic and correlation



Magic and correlation

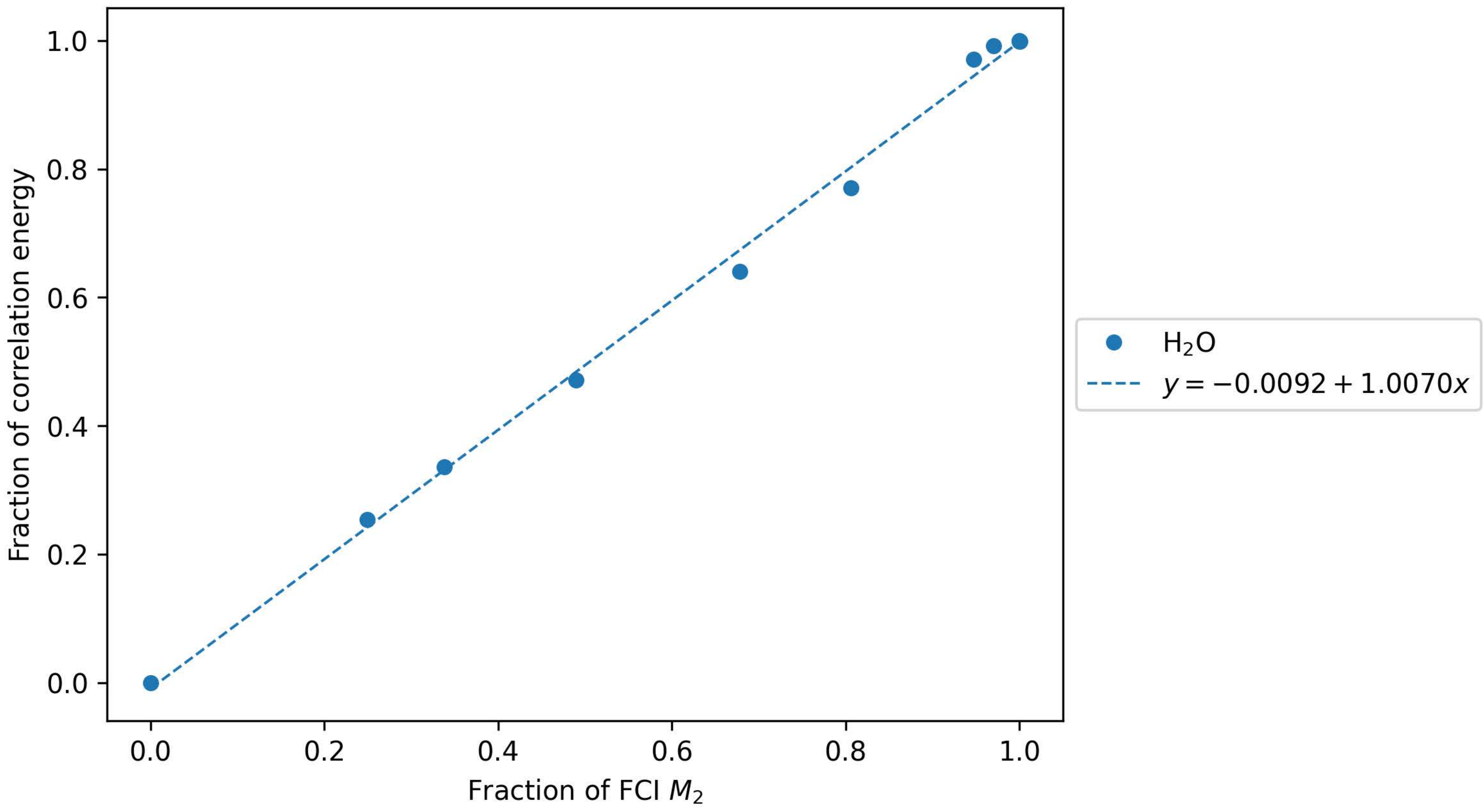




How more correlation energy we gain seems to change with how much magic we've gained

Magic and correlation

Correlation energy grows **linearly** with the amount of magic we've added to our ground state!



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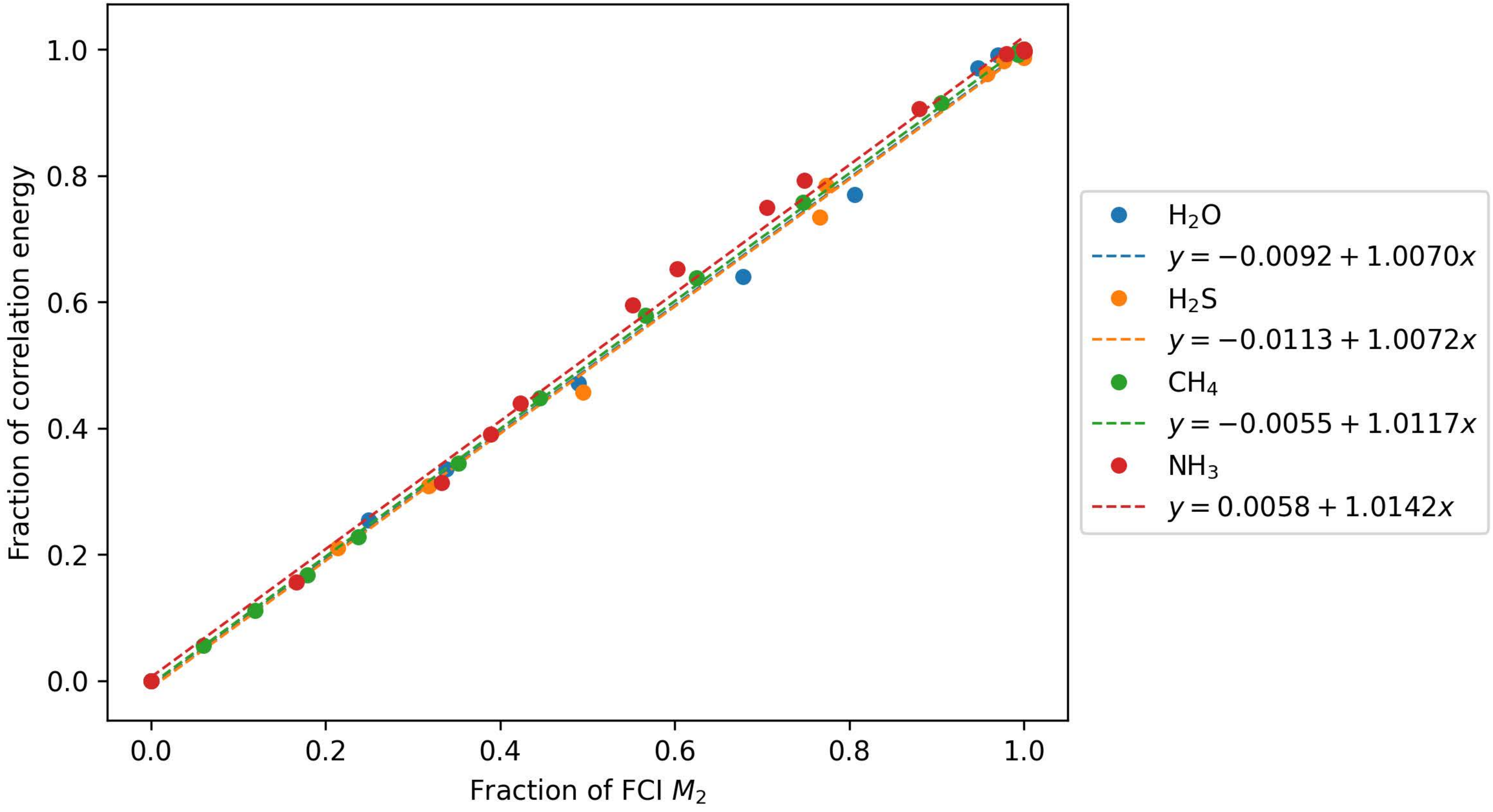
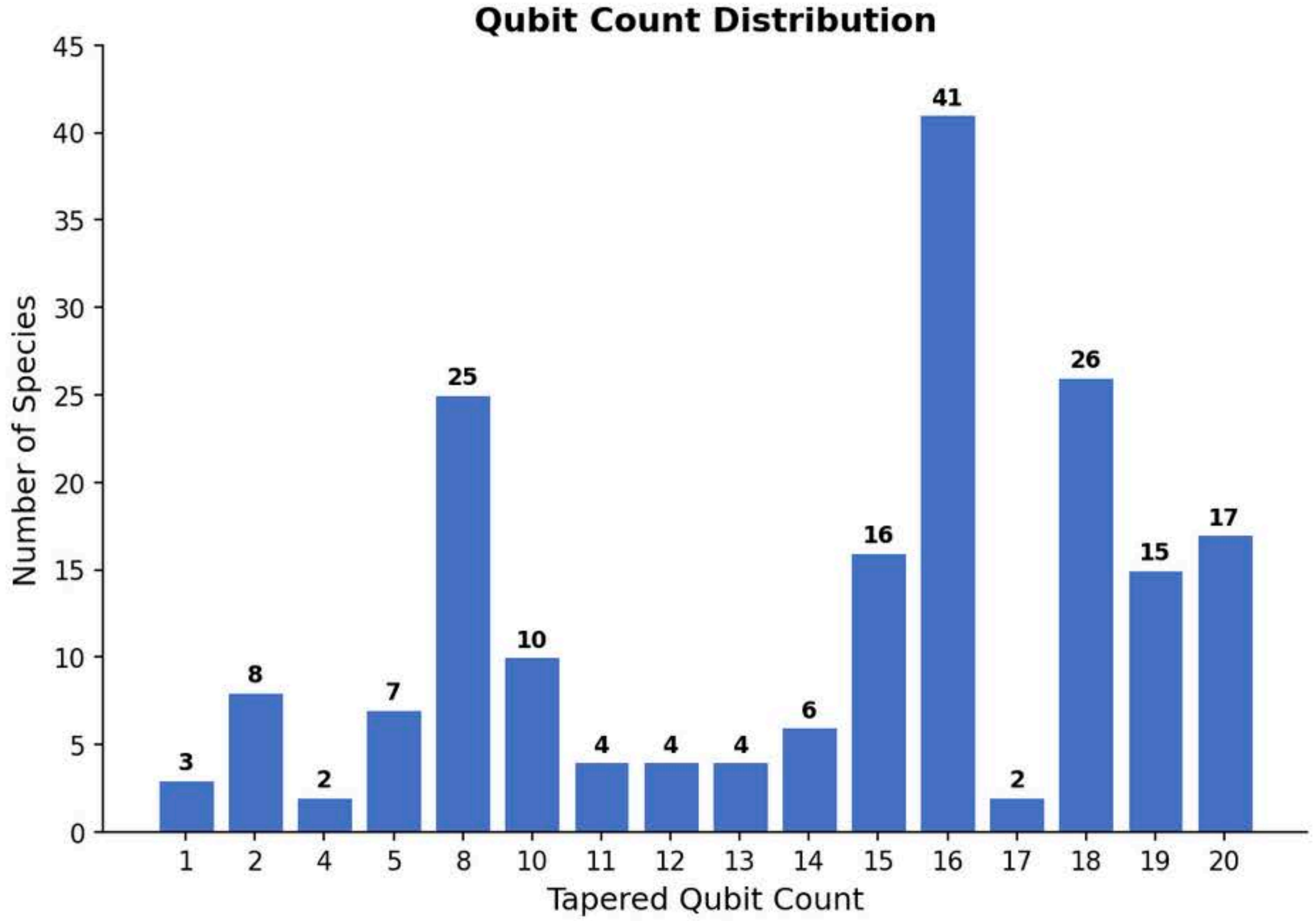
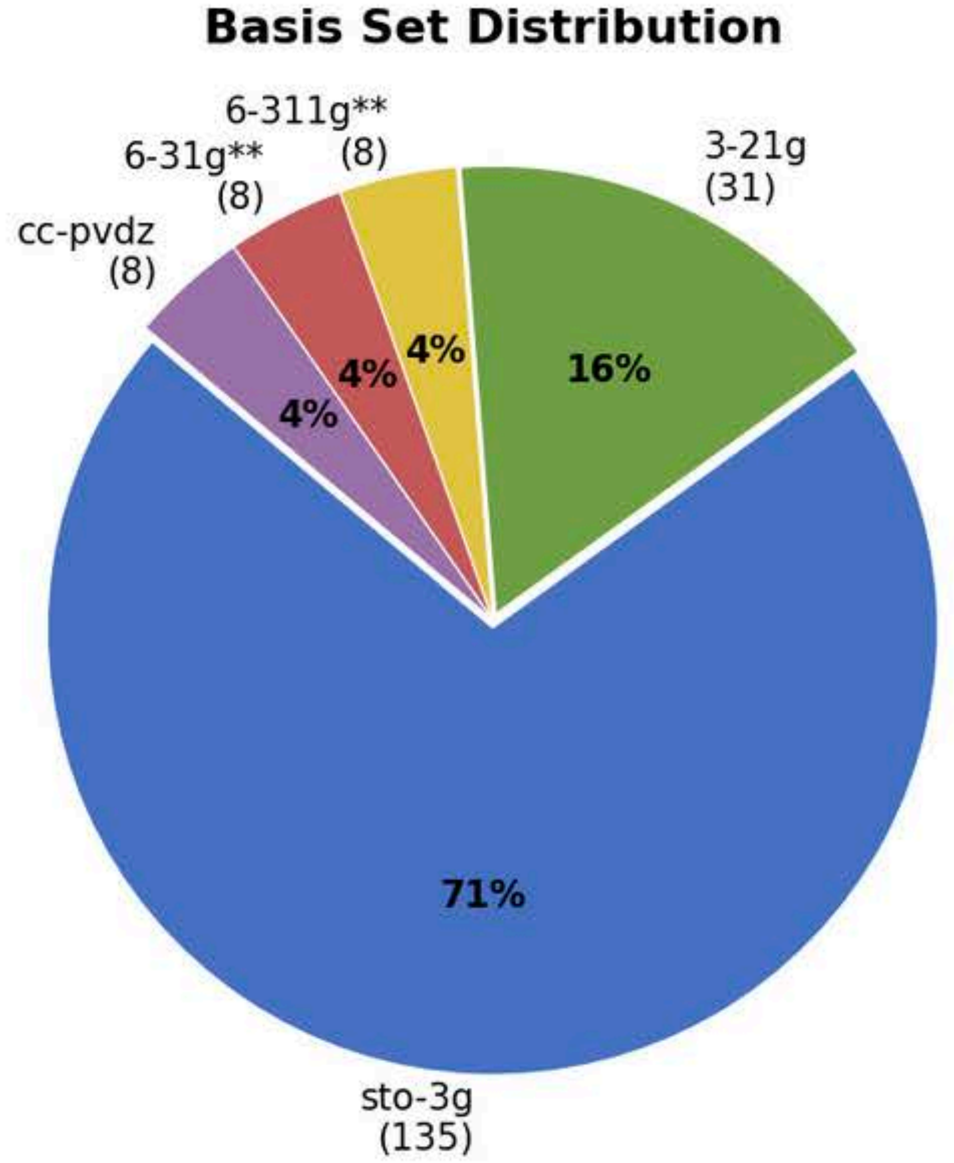


Hamilton data set

Symmer-Hamiltonian

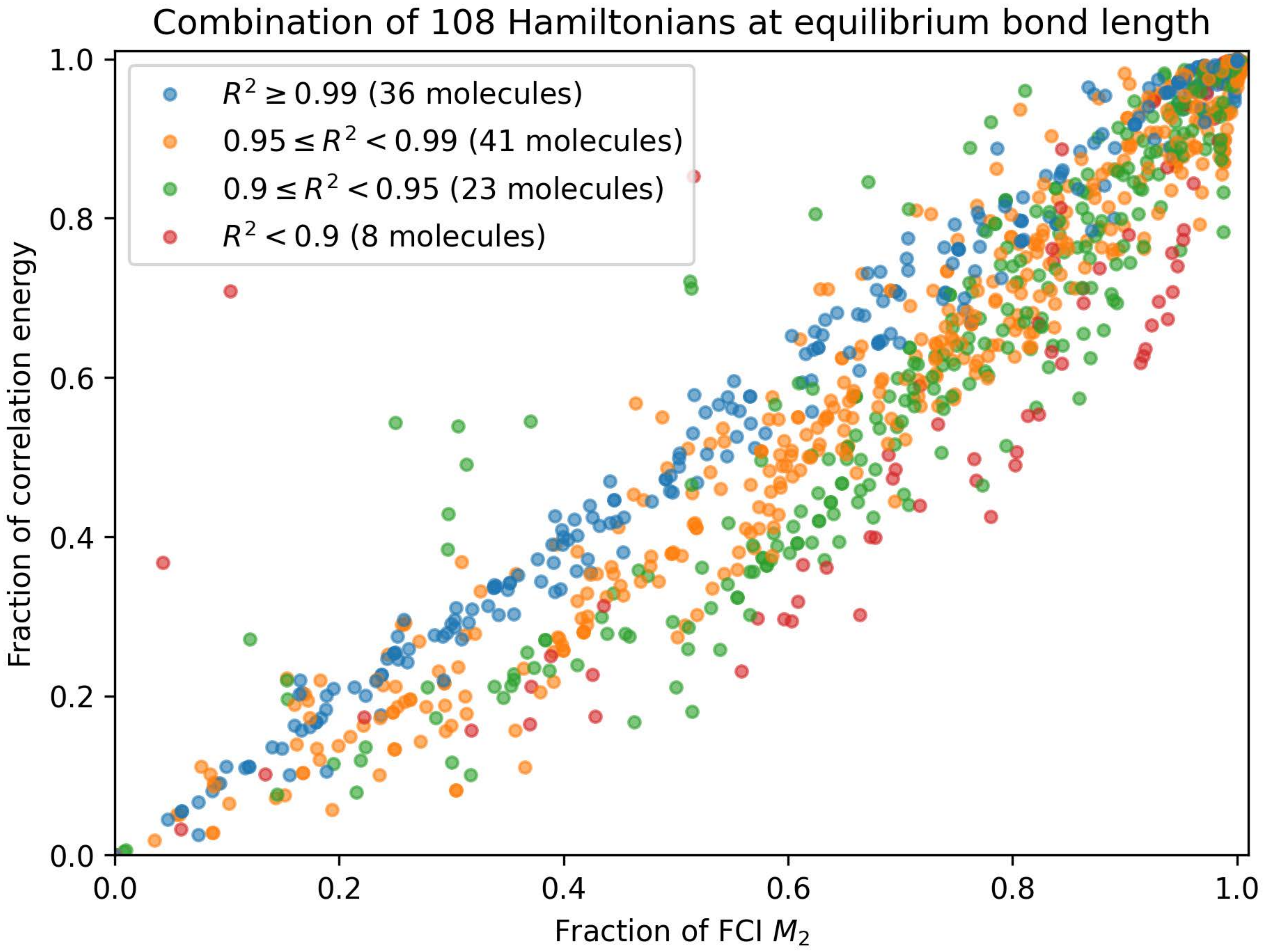
A curated database of molecular electronic Hamiltonians in Symmer-compatible qubit (Pauli operator) form, generated using the symmer-pyscf pipeline.

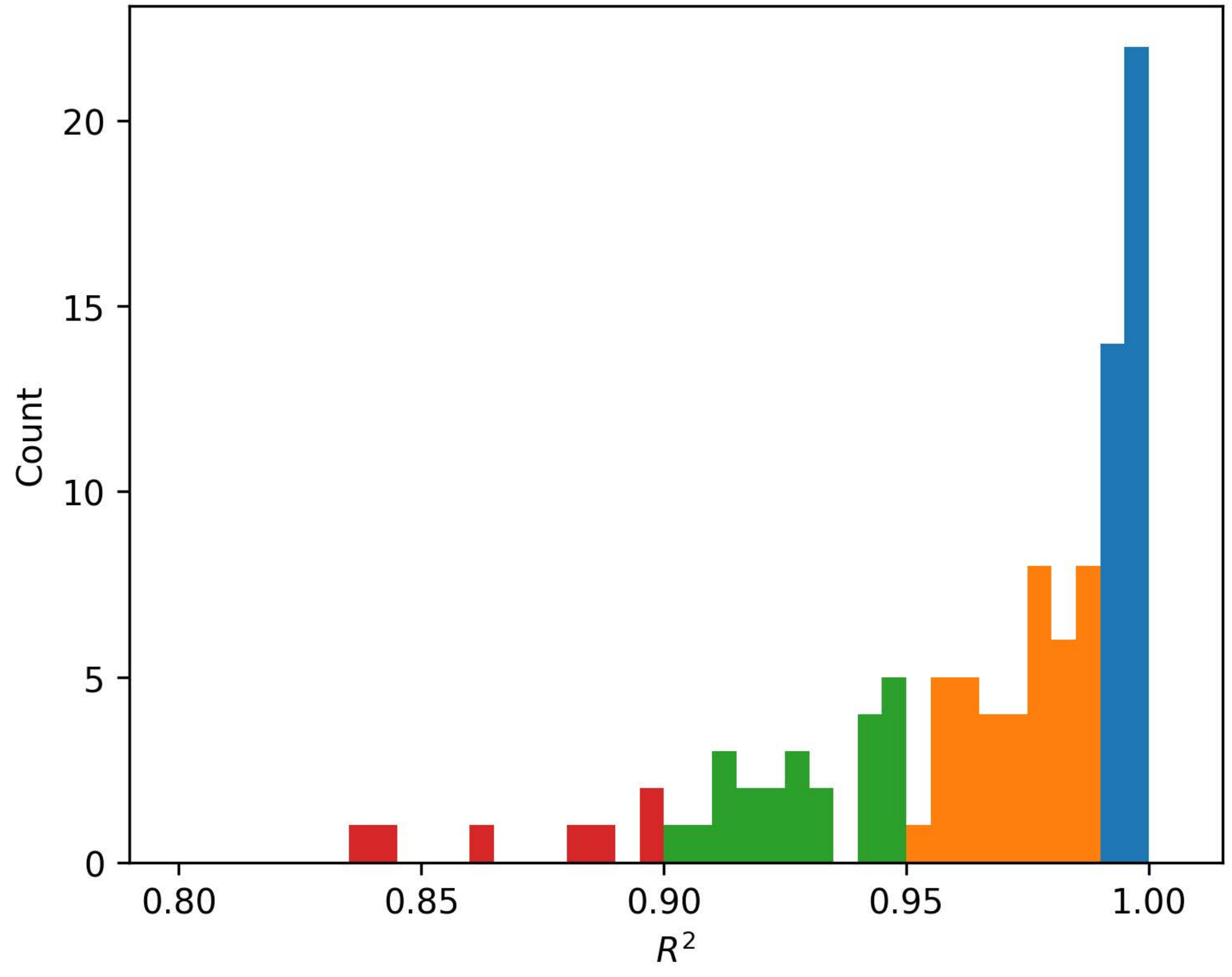




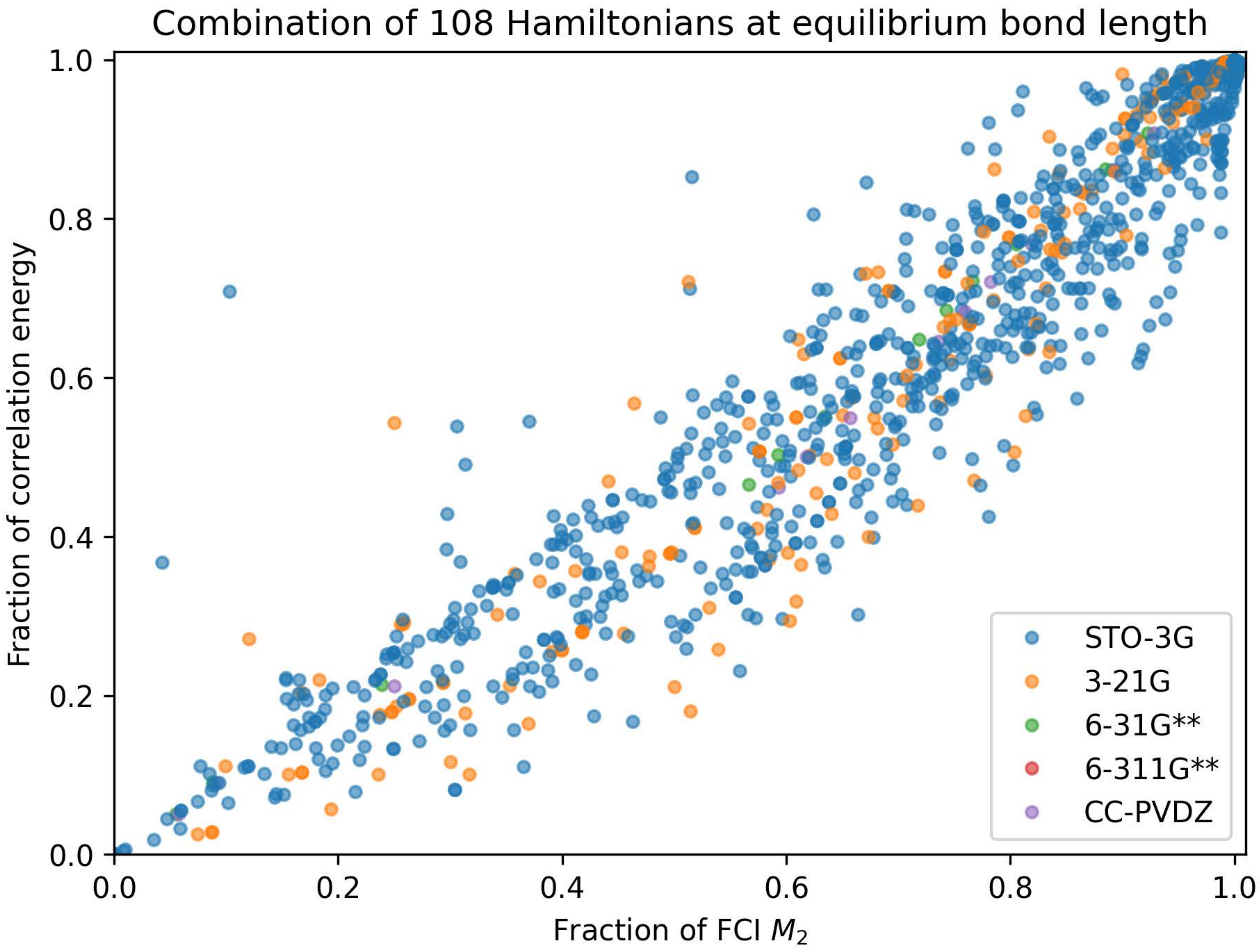
github.com/Kee-Wang/Symmer-Hamiltonian

Magic and correlation

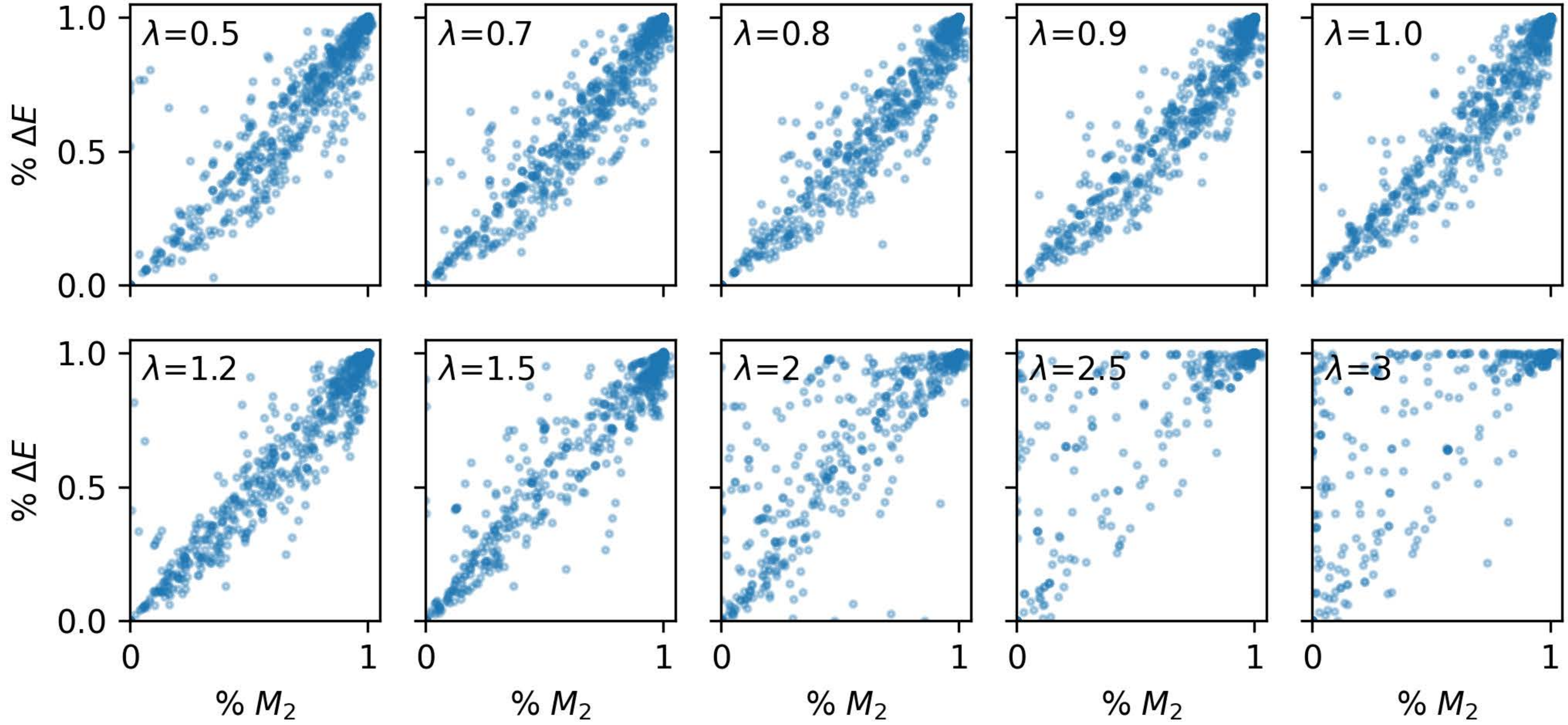




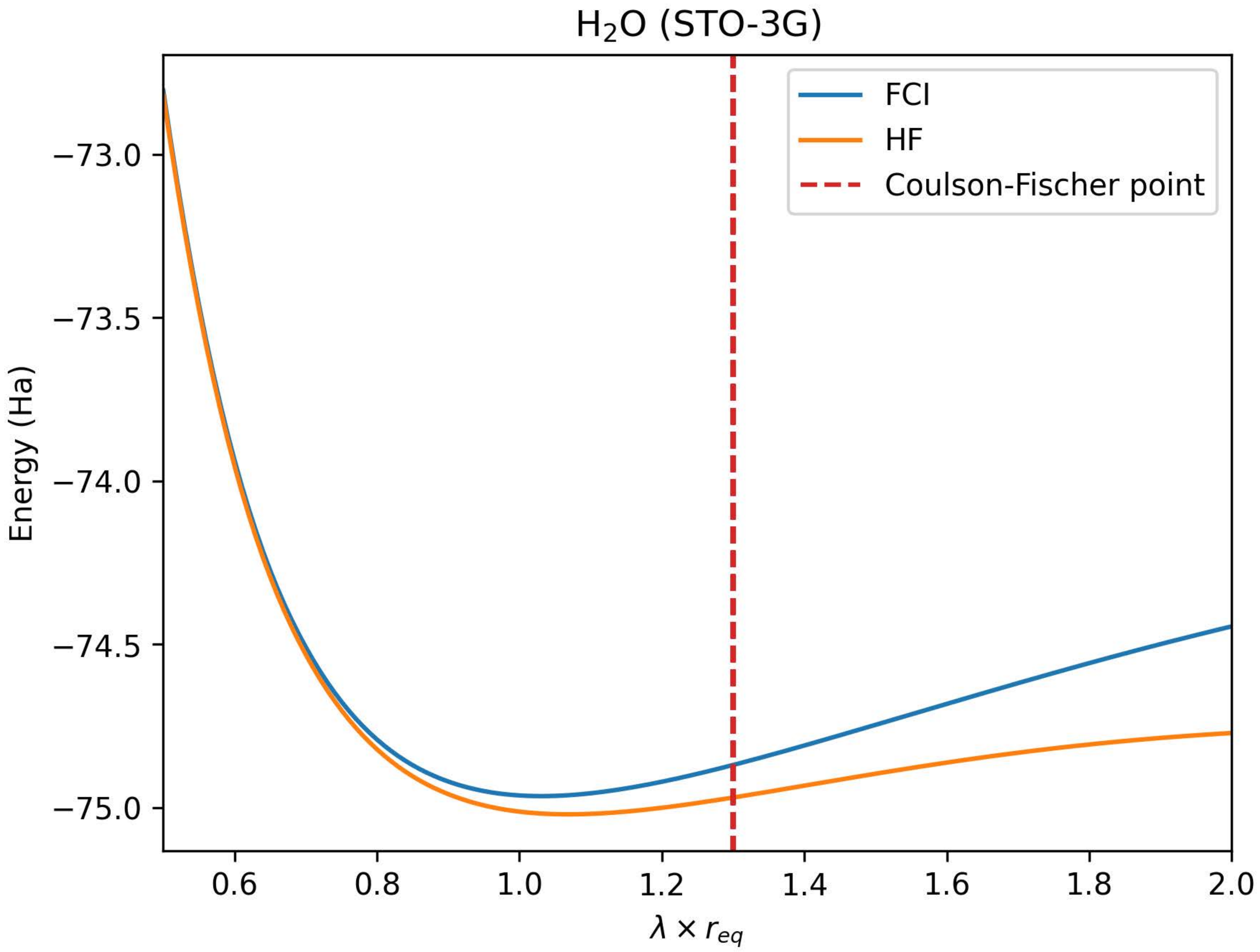
Magic and correlation energy: does the basis set matter?



Magic and correlation: away from equilibrium



The Coulson-Fischer point

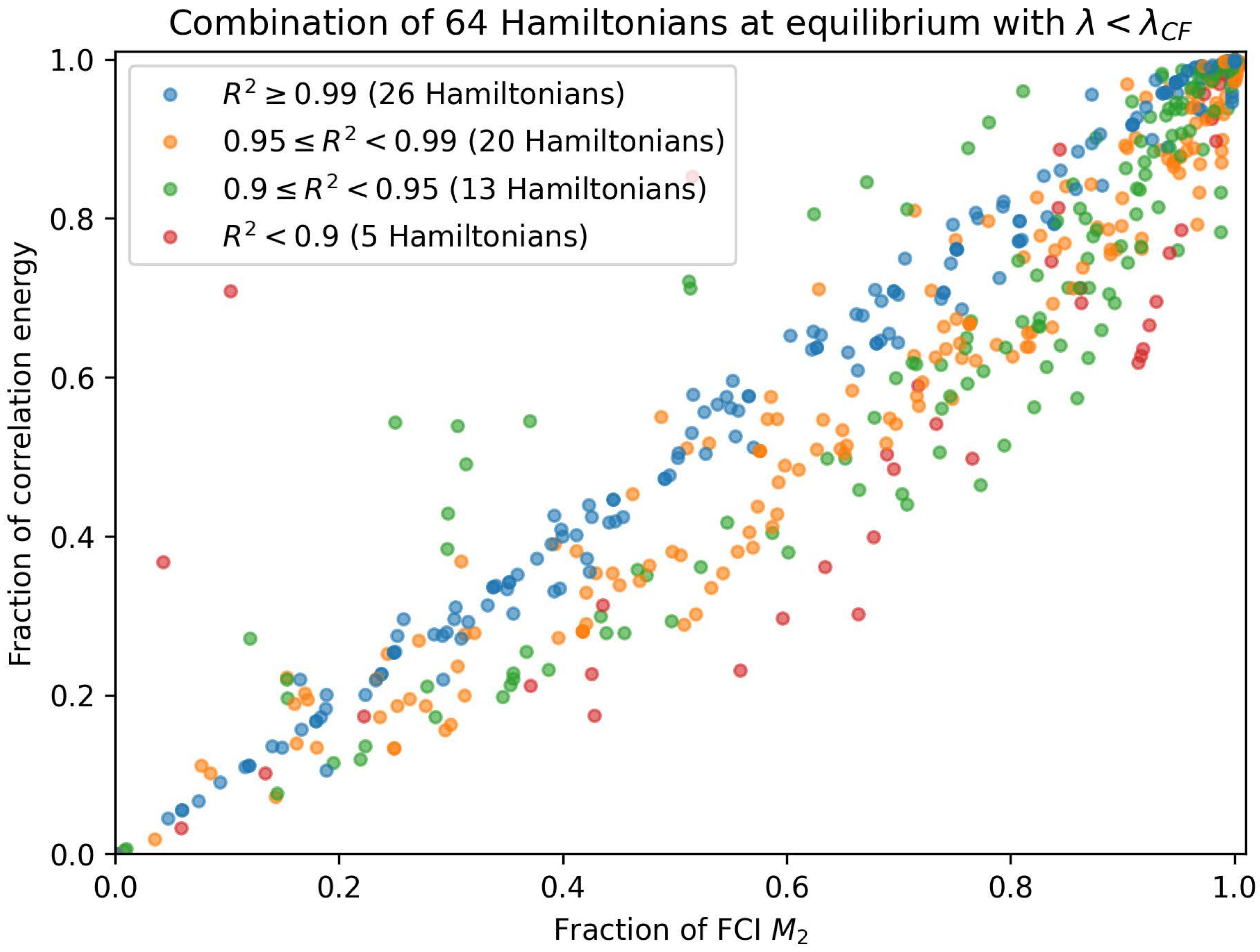


Hartree-Fock gets less accurate as bond length increases

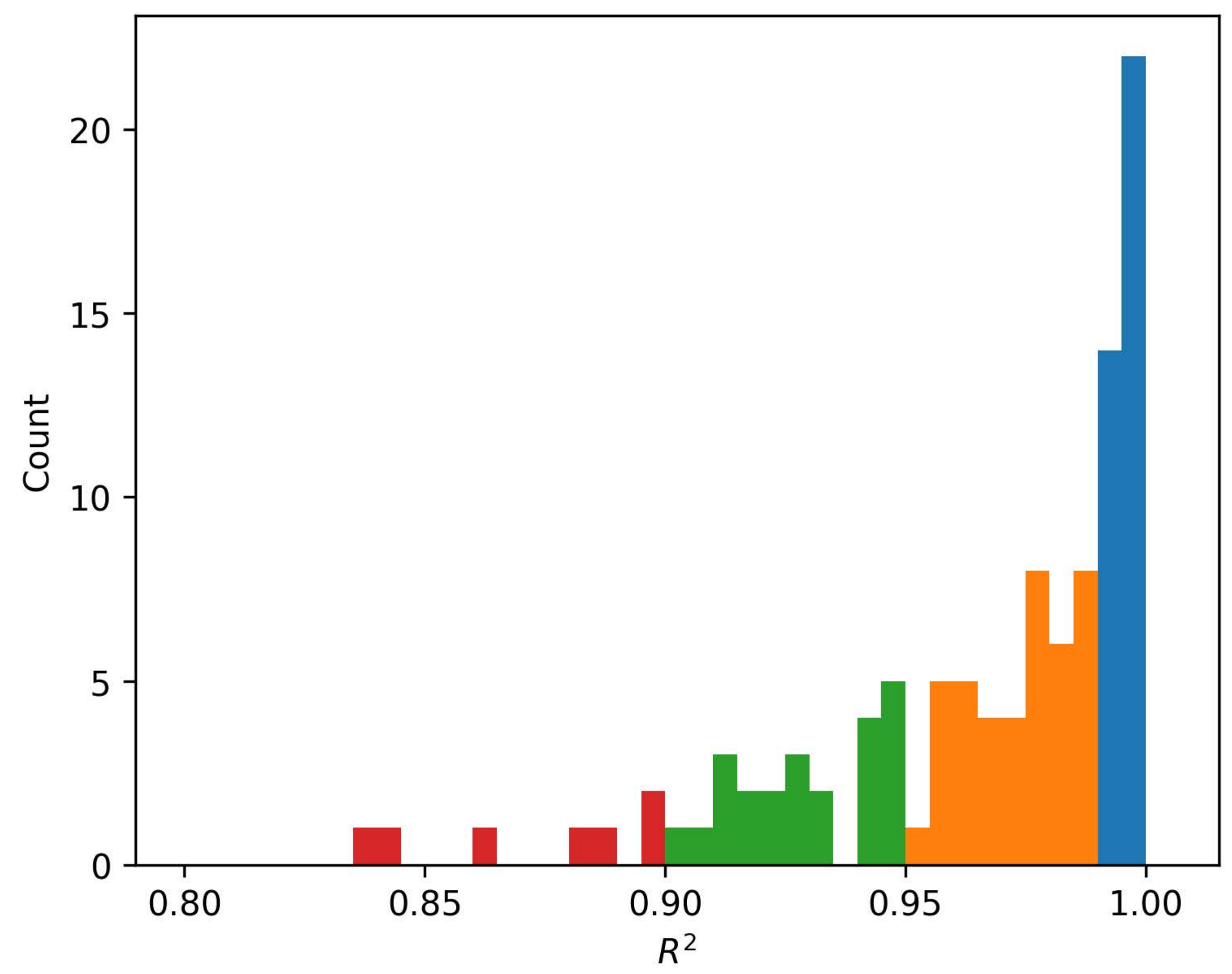
Beyond the **Coulson-Fischer point**, Hartree-Fock no longer gives the best mean-field approximation

C. A. Coulson and I. Fischer. "Notes on the molecular orbital treatment of the hydrogen molecule." *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science* **40.303** (1949): 386-393.

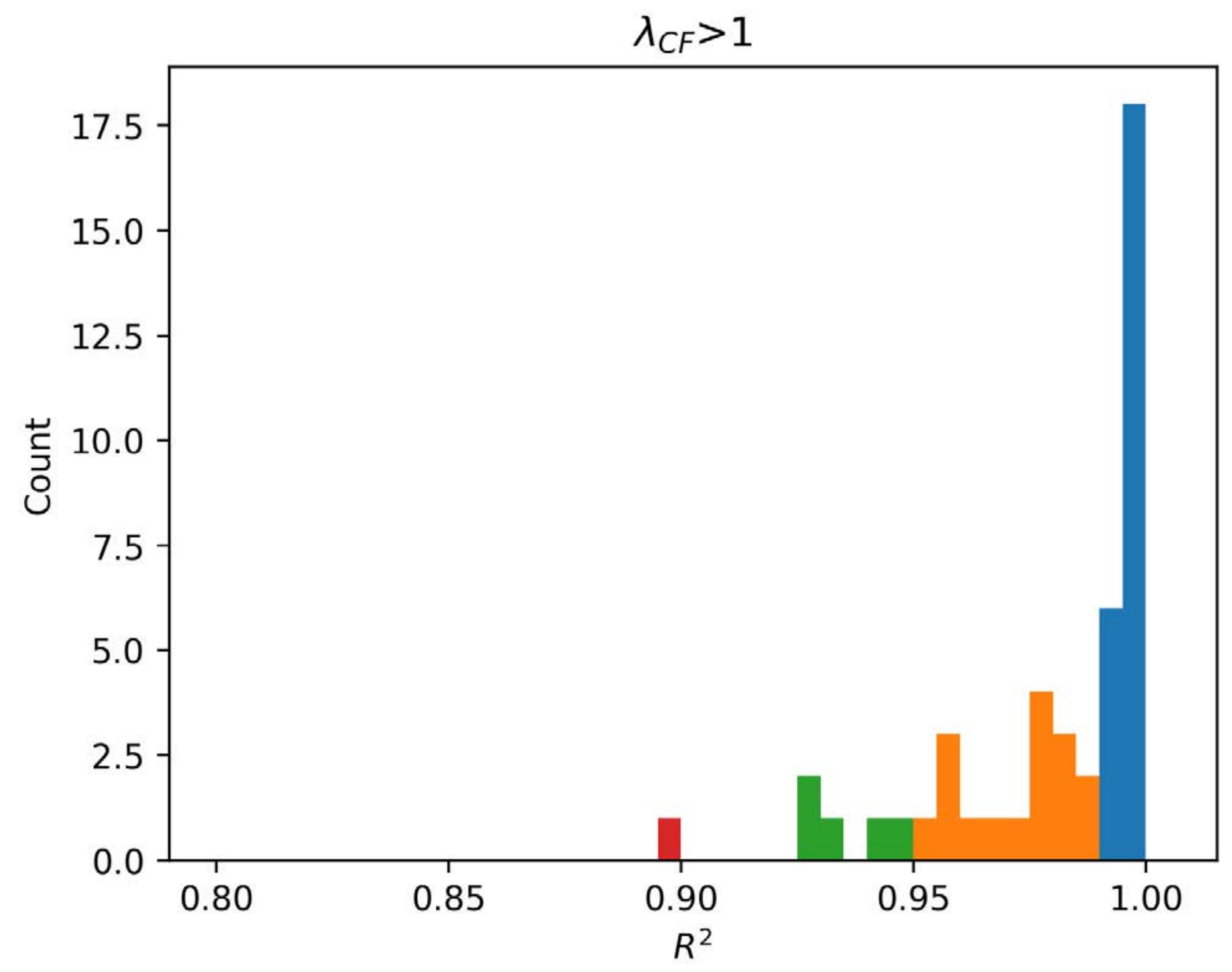
The Coulson-Fischer point



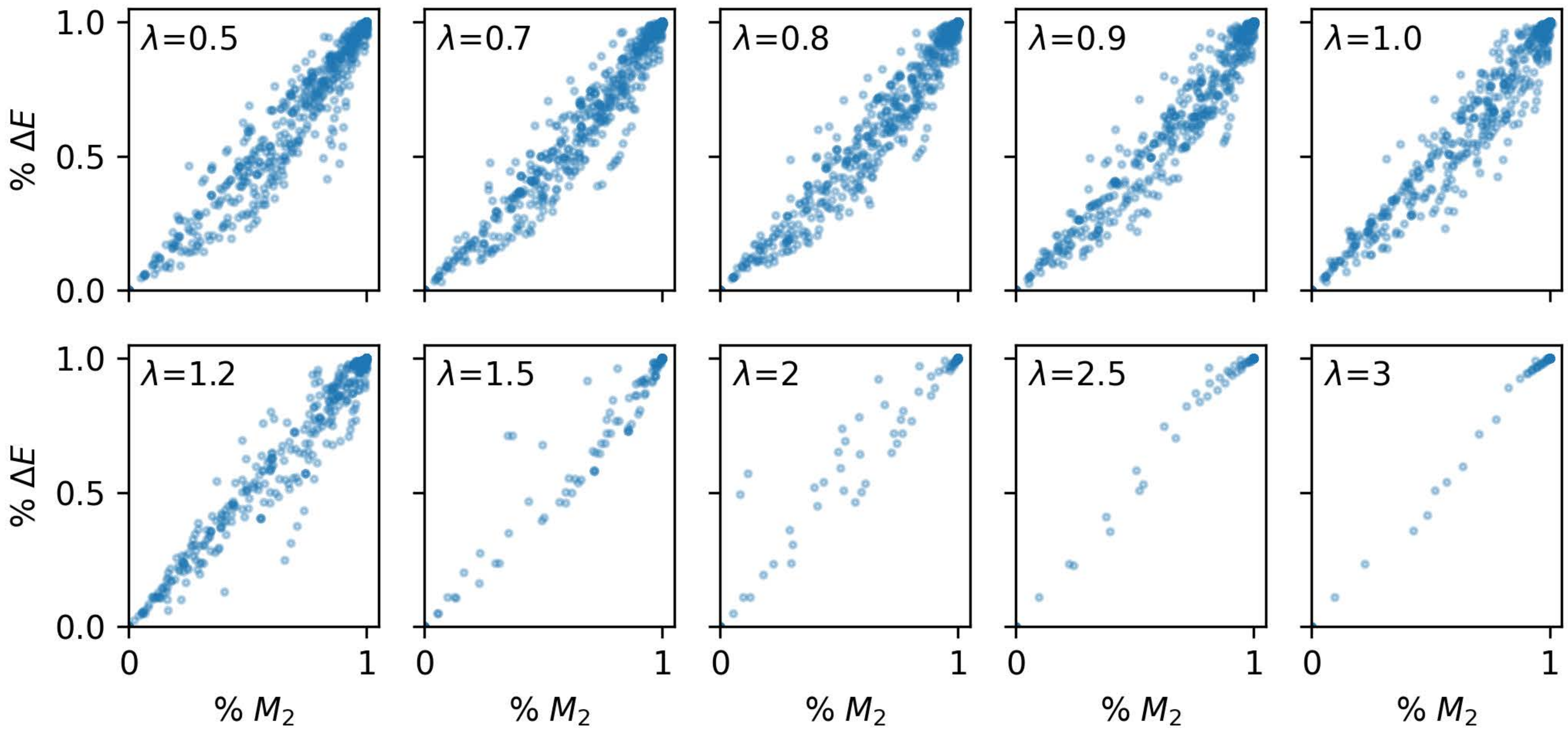
Including all molecules

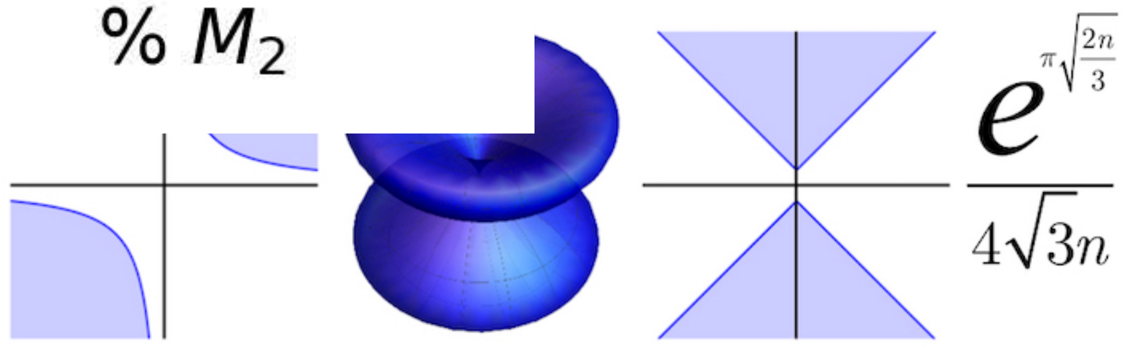


Limit to $\lambda_{CF} > 1$



Magic and correlation: away from equilibrium





Conclusions

- Noncontextual Hamiltonians provide a natural setting in which states with bounded stabilizer rank occur.

- They are “short range magic” Hamiltonians - are they the only ones?

- Many applications in Chemistry where noncontextual H replaces Hartree-Fock, changing definition of correlation energy.

- Current work - can we use contextual subspace method to identify subspaces where physical intuition does not help, particularly in no core shell model?

- Can we extend this formalism beyond Pauli operators, to general sparse Hamiltonians?

Thanks!

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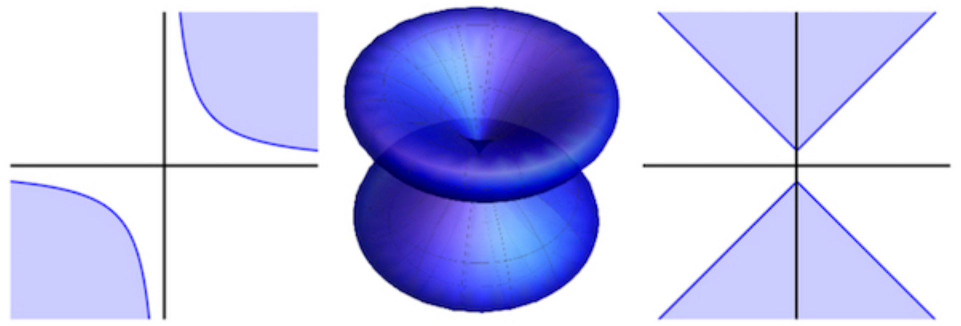

$$\frac{e^{\pi\sqrt{\frac{2n}{3}}}}{4\sqrt{3}n}$$