Minimizing State Preparations for VQE

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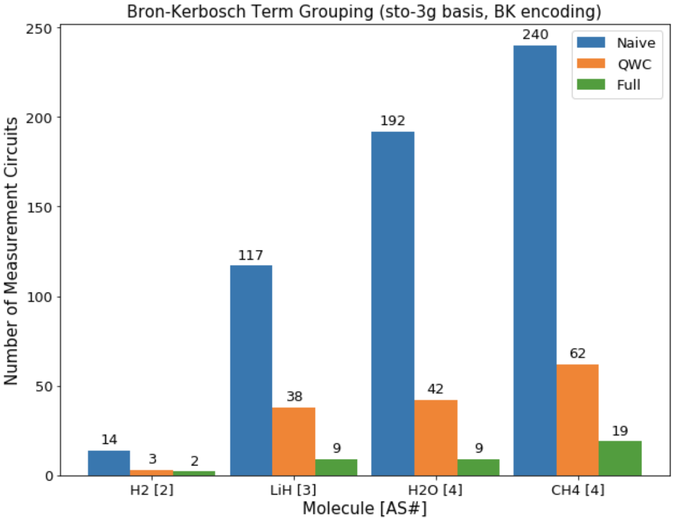
EPiQC: Enabling Practical-scale Quantum Computation

QRE 2019, June 22

Results



Bron-Kerbosch Term Grouping (sto-3g basis, BK encoding)
Number of Measurement Circuits
Molecule [AS#]
Naive
QWC
Full
0
50
100
150
200
250
14
3
2
117
38
9
192
42
9
240
62
19
H2 [2]
LiH [3]
H2O [4]
CH4 [4]

Background: Ground State Estimation

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- Classically, diagonalize exponentially-sized matrix.
- Quantum Phase Estimation algorithm showed how to solve in poly-time.

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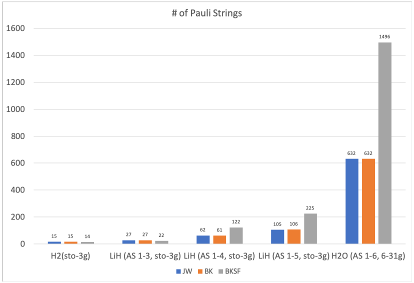

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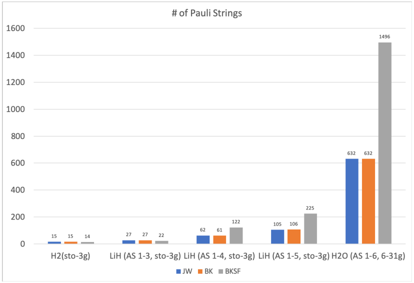

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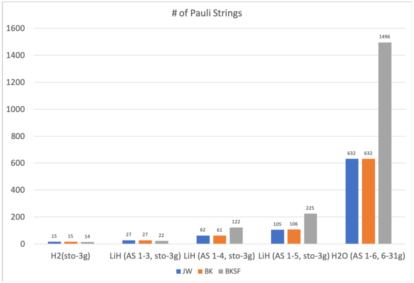

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- Impact on variance and study of covariances
- Benchmarking & resource estimation for representative molecules

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Commutator Notation

$$[A, B] = AB - BA \begin{cases} = 0 & \text{if } A \text{ and } B \text{ commute} \\ \neq 0 & \text{if } A \text{ and } B \text{ do not commute} \end{cases}$$

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In general: QWC simultaneous measurements requires $O(N)$ single qubit gates (depth $= 1$).

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Proof: All Pauli strings are either commuting or anti-commuting, so we know that either $AB = BA$ or $AB = -BA$. Each commuting index multiplies by $+1$, each non-commuting index multiplies by -1. Need even number of non-commuting indices to have a total $+1$.

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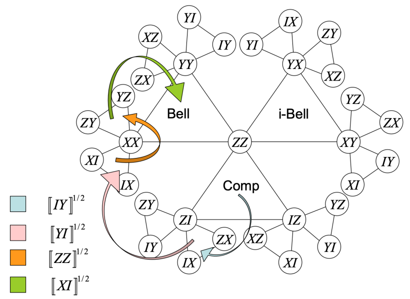

[Devoret Notes]

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$O(N^2)$ gates is fine, because UCCSD ansatz prep is $O(N^3)$ or $O(N^4)$.

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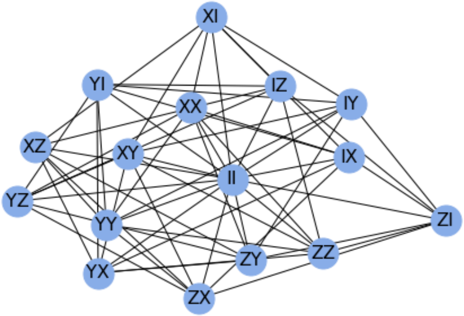

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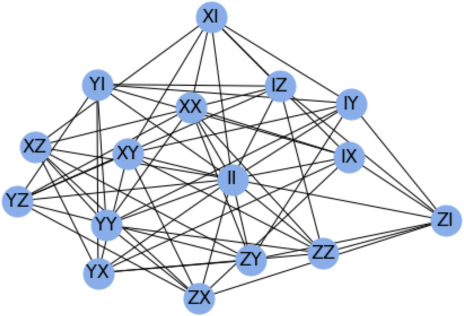

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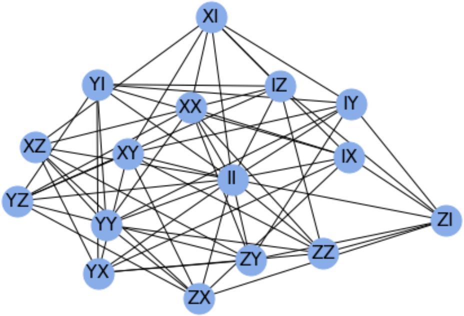

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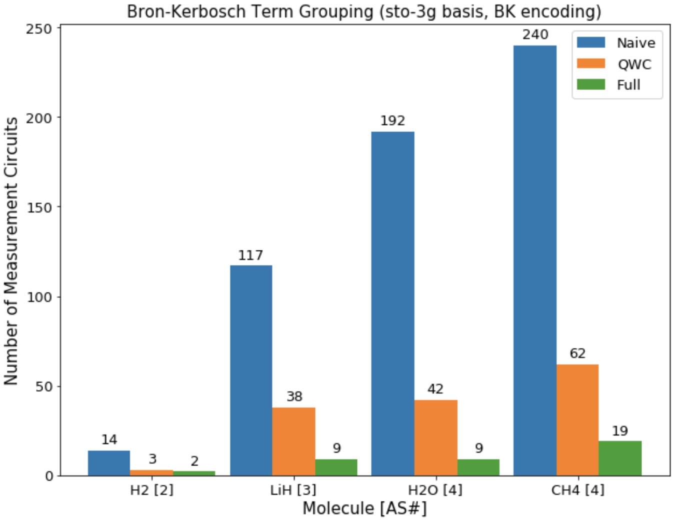
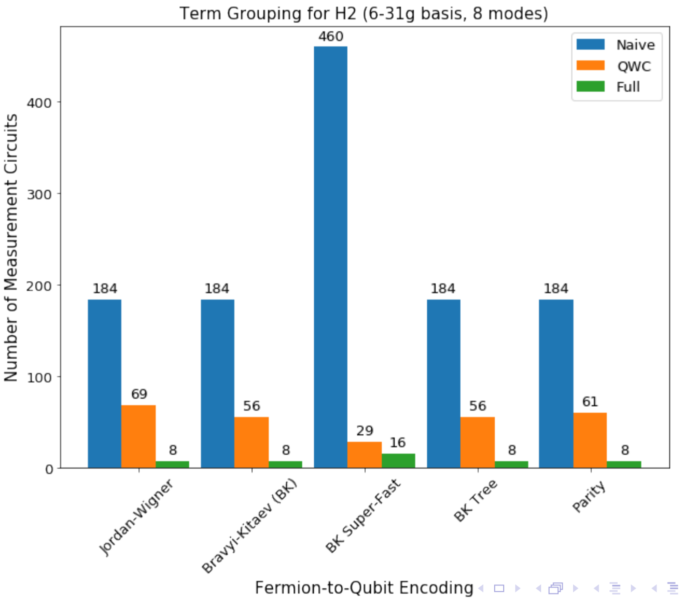
Problem is NP-Hard, but use heuristics (Boppana-Halldórsson). Note that our problem is also NP-HARD by reduction from MIN-CLIQUE-COVER.

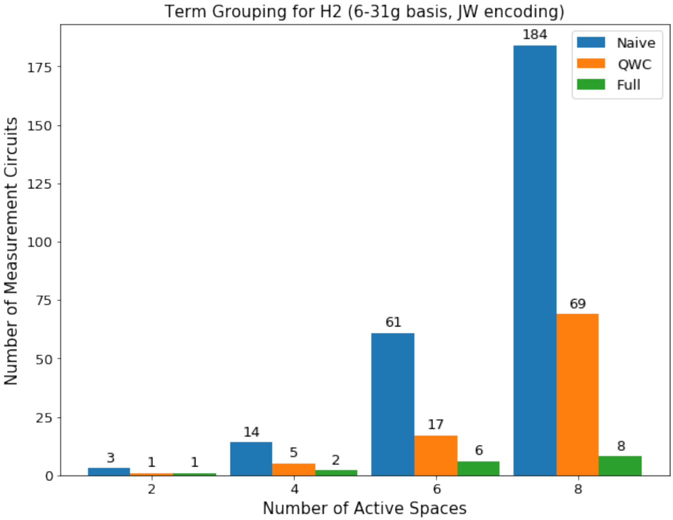
Results: Across Molecules



Results: Across Encodings



Results: Across Active Spaces



Qubit Tapering

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σ_1^z	σ_2^z	σ_3^z	σ_4^z
$\sigma_1^z\sigma_2^z$	$\sigma_1^z\sigma_3^z$	$\sigma_1^z\sigma_4^z$	
$\sigma_2^z\sigma_3^z$	$\sigma_2^z\sigma_4^z$	$\sigma_3^z\sigma_4^z$	
$\sigma_1^y\sigma_2^y\sigma_3^x\sigma_4^x$	$\sigma_1^x\sigma_2^y\sigma_3^y\sigma_4^x$	$\sigma_1^y\sigma_2^x\sigma_3^x\sigma_4^y$	$\sigma_1^x\sigma_2^x\sigma_3^y\sigma_4^y$

$$U_1 = \frac{1}{\sqrt{2}}\left(\sigma_2^x + \sigma_1^z\sigma_2^z\right), \quad U_2 = \frac{1}{\sqrt{2}}\left(\sigma_3^x + \sigma_1^z\sigma_3^z\right)$$

and $U_3 = \frac{1}{\sqrt{2}}\left(\sigma_4^x + \sigma_1^z\sigma_4^z\right).$

$\longrightarrow$

σ_1^z	$\sigma_1^z\sigma_2^x$	$\sigma_1^z\sigma_3^x$	$\sigma_1^z\sigma_4^x$
σ_2^x	σ_3^x	σ_4^x	
$\sigma_2^x\sigma_3^x$	$\sigma_2^x\sigma_4^x$	$\sigma_3^x\sigma_4^x$	
$\sigma_1^x\sigma_3^x\sigma_4^x$	$\sigma_1^x\sigma_4^x$	$\sigma_1^x\sigma_2^x\sigma_3^x$	$\sigma_1^x\sigma_2^x$

- In example, three qubits are tapered out of H2 Hamiltonian

Qubit Tapering Results

Hamiltonian	# of Qubits	# Tapered
H2 (small # active spaces)	4	3
H2 (large # active spaces)	8	2
H2O	8	2

Measurement Statistics[1]

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Example

Consider $H = -XX - YY + ZZ + IZ + ZI$, and state $|\psi\rangle = |01\rangle$.

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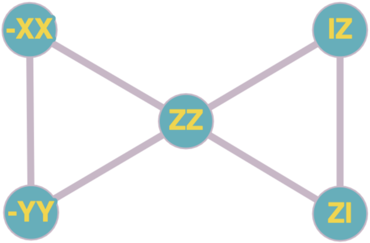

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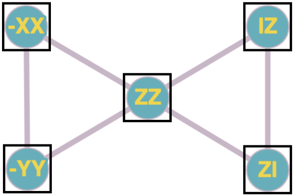

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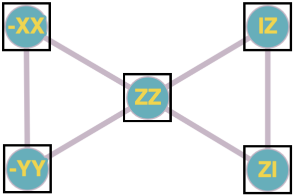


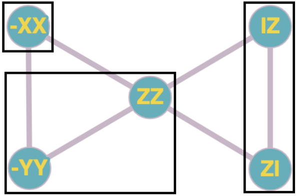
$$E(\#\text{ state preps}) =$$

$$k\Big(Var(-XX) + Var(-YY) + Var(ZZ) + Var(ZI) + Var(IZ)\Big)/\epsilon^2$$

$$= 5\Big(1 + 1 + 0 + 0 + 0\Big)/\epsilon^2$$

$$= \boxed{10/\epsilon^2}$$

$k = 3$ Groups



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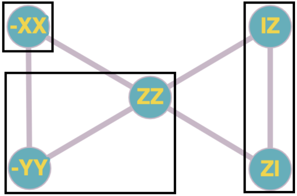


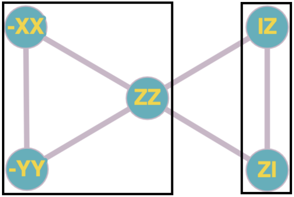
$$E(\#\text{ state preps})/\epsilon^2 =$$

$$k\Big[Var(-XX) + Var(\{-YY, -ZZ\}) + Var(\{ZI, IZ\})\Big]/\epsilon^2$$

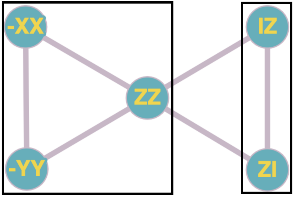
$$= k\Big[Var(-XX) + \Big(Var(-YY) + Var(-ZZ) + 2Cov(-YY, -ZZ)\Big) + \Big(Var(ZI) + Var(IZ) + 2Cov(IZ, ZI)\Big)\Big]/\epsilon^2$$

$$= 3\Big[1 + \Big(1 + 0 + 0\Big) + \Big(0 + 0 + 0\Big)\Big]/\epsilon^2 = \boxed{6/\epsilon^2}$$

$k = 2$ Groups



$k = 2$ Groups



$$E(\#\text{ state preps}) =$$

$$k\Big[Var(\{-XX, -YY, ZZ\}) + Var(\{ZI, IZ\})\Big]/\epsilon^2$$

$$= k\Big[\Big(Var(-XX) + Var(-YY) + Var(ZZ) +$$

$$2Cov(-XX, -YY) + 2Cov(-XX, ZZ) + 2Cov(-YY, ZZ)\Big)$$

$$\Big(Var(ZI) + Var(IZ) + 2Cov(IZ, ZI)\Big)\Big]/\epsilon^2$$

$$= 2\Big[\Big(1 + 1 + 0 + 2 * 1 + 0 + 0\Big) + \Big(0 + 0 + 0\Big)\Big]/\epsilon^2 = \boxed{8/\epsilon^2}$$

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Work in progress: adaptively adjust groups after initial grouping.

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