

Preparing Bethe ansatz states and other interesting many-body states on a quantum computer

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Classical simulations of quantum systems

In general, representing n quantum 2-level systems involves storing $2 * 2^n$ real numbers. Scaling is **exponential!**

Even storing moderately-sized quantum states is infeasible with classical hardware

# of qubits	RAM required to store state
1	32 B
10	16 kiB
20	16 MiB
30	16 GiB
40	16 TiB
46	1 PiB

Quantum simulation

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

International Journal of Theoretical Physics, Vol. 21, p. 467 (1982)

- Size of Hilbert space grows exponentially with system size
→ Inefficient to store wavefunctions on classical computers
- Use quantum devices to simulate other quantum systems

Analog vs digital simulation

- **Analog quantum simulation**
 - Create Hamiltonian of system on simulator
 - Simulator has tunable parameters, study various regimes
 - Limited by native interactions of simulator
- **Digital quantum simulation**
 - Evolution decomposed into elementary gates
 - Any problem can in principle be solved
 - Need to map problem to quantum processor
(straightforward with spin $\frac{1}{2}$ lattice models)

Mapping fermionic problems to qubits

- Fermionic Hamiltonian

$$\hat{H} = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

Jordan-Wigner mapping:

- Each orbital is mapped onto a qubit: $|0\rangle \rightarrow$ unoccupied orbital, $|1\rangle \rightarrow$ occupied orbital

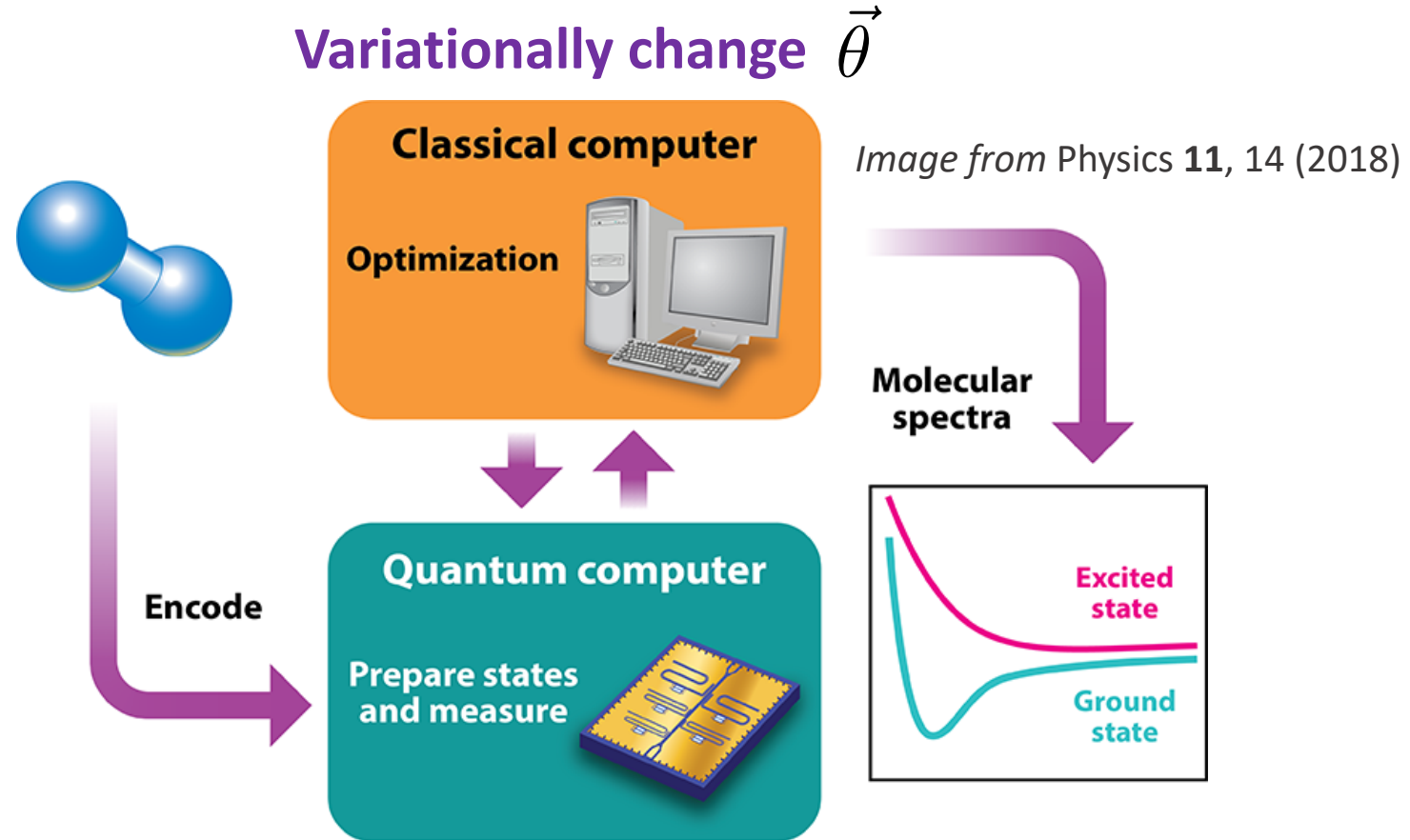
$$a_3^\dagger |1001\rangle = a_3^\dagger a_1^\dagger a_4^\dagger |0000\rangle = -a_1^\dagger a_3^\dagger a_4^\dagger |0000\rangle$$

- Fermions satisfy Pauli exclusion principle but qubits are distinguishable \rightarrow impose on qubits through Z strings

$$a_i^\dagger = \frac{1}{2} (X_i - iY_i) \otimes_{j<i} Z_j$$

Variational quantum eigensolver (VQE) algorithms

Nat. Comm. **5**, 4213 (2014)
New J. Phys. **18**, 023023 (2016)
arXiv:2012.09265 (2021)



Ansatz

$$|\Psi(\vec{\theta})\rangle = T(\vec{\theta})|\Psi_{ref}\rangle$$

Measured energy

$$E(\vec{\theta}) = \langle \Psi(\vec{\theta}) | H | \Psi(\vec{\theta}) \rangle$$

Cost function and wavefunction ansatz

$$C(\vec{\theta}) = \langle \Psi(\vec{\theta}) | H | \Psi(\vec{\theta}) \rangle \quad |\Psi(\vec{\theta})\rangle = T(\vec{\theta}) |\Psi_{ref}\rangle$$

Commonly used ansätze:

Hardware-efficient ansatz

- Use gates native to hardware
- Inefficient—too much of the Hilbert space sampled
- Difficult to optimize (barren plateaus)
McClean et al., Nat. Commun. 9, 4812 (2018)

Chemistry-inspired ansatz (UCC)

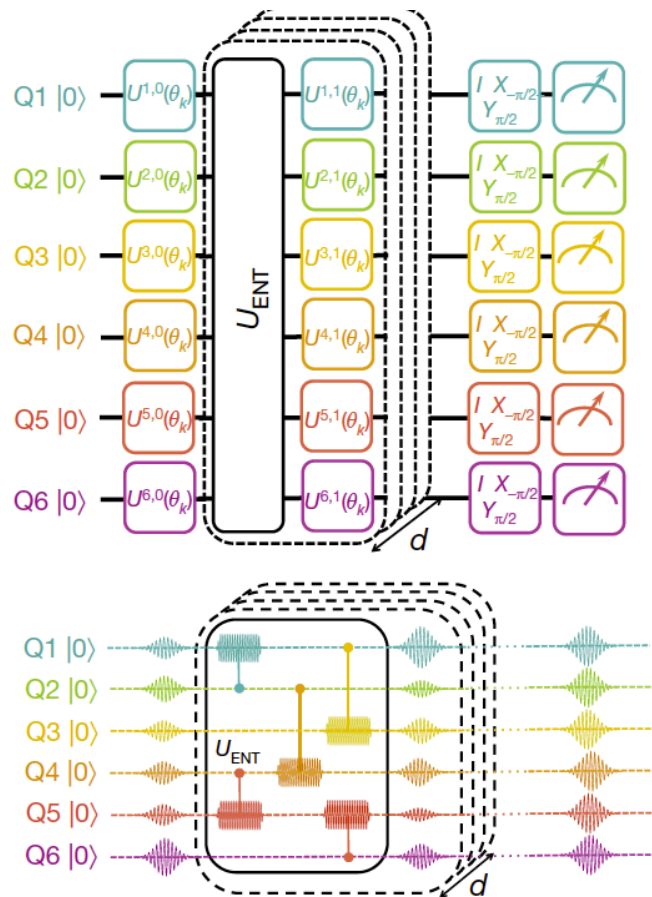
- Respects symmetries of problem
- State preparation times exceed coherence times
- Not guaranteed to be exact
- Ill-defined under low-order Trotterization

Grimsley et al., JCTC 2020, 16, 1, 1-6

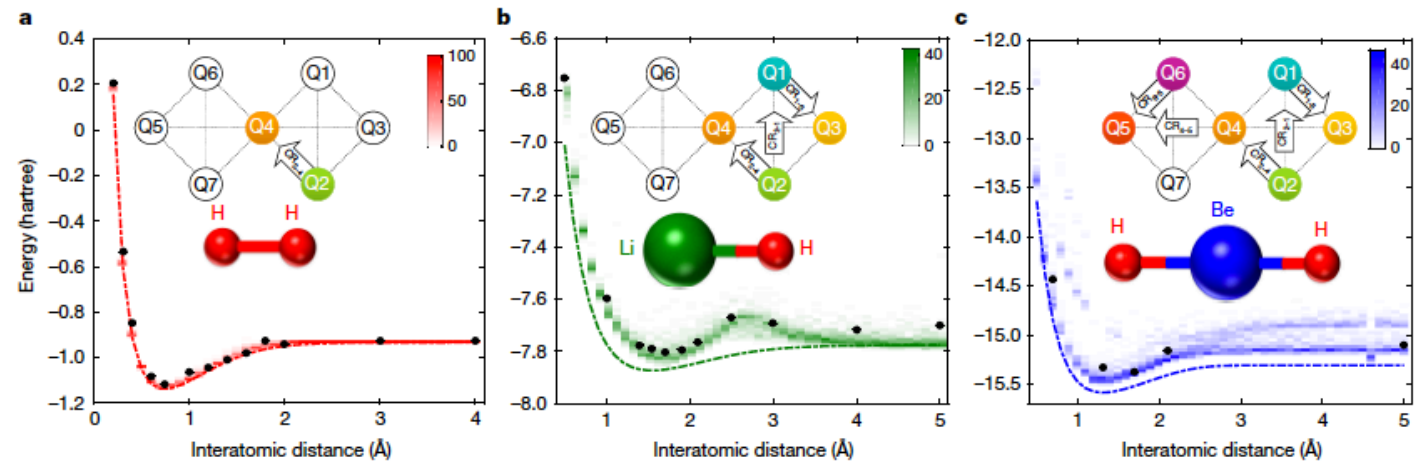
Both approaches use very little information from problem Hamiltonian

Experiments using hardware-efficient ansätze

- Alternating gate structure
- Single-qubit gates contain optimized parameters

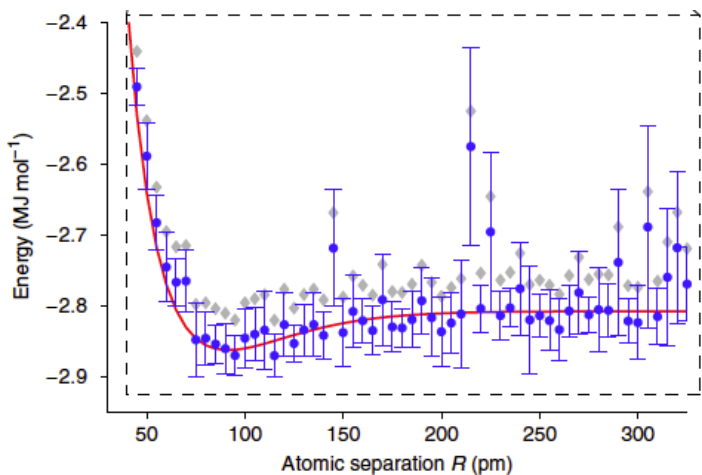


Kandala et al (IBM group), Nature **549**, 242 (2017)



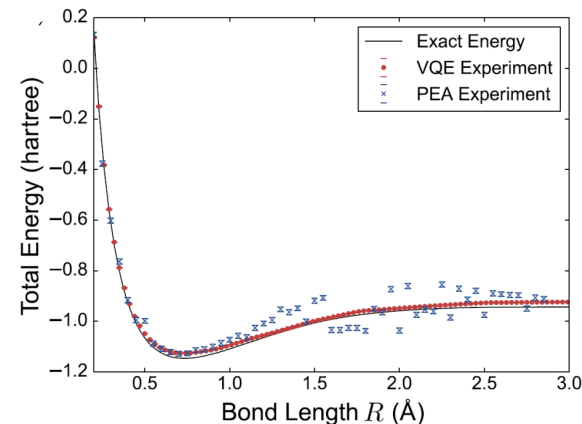
Experiments using chemistry-inspired ansätze (UCCSD)

- Photonic qubits, He-H⁺ ground state



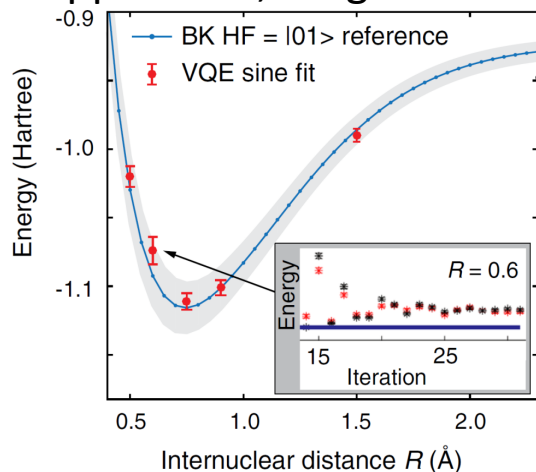
*Peruzzo et al,
Nature Comm. 5, 1 (2014)*

- Superconducting qubits, H₂ ground state



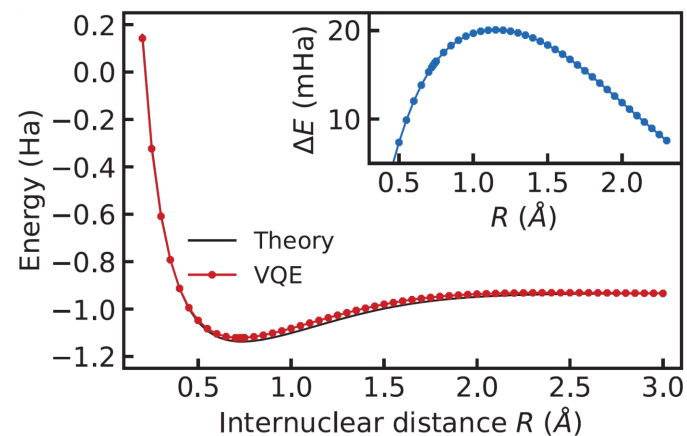
*O'Malley et al,
PRX 6, 031007 (2016)*

- Trapped ions, H₂ ground state



*Hempel et al,
PRX 8, 031022 (2018)*

- Spin qubits, H₂ ground state



*Xue et al,
Nature 601, 343 (2022)*

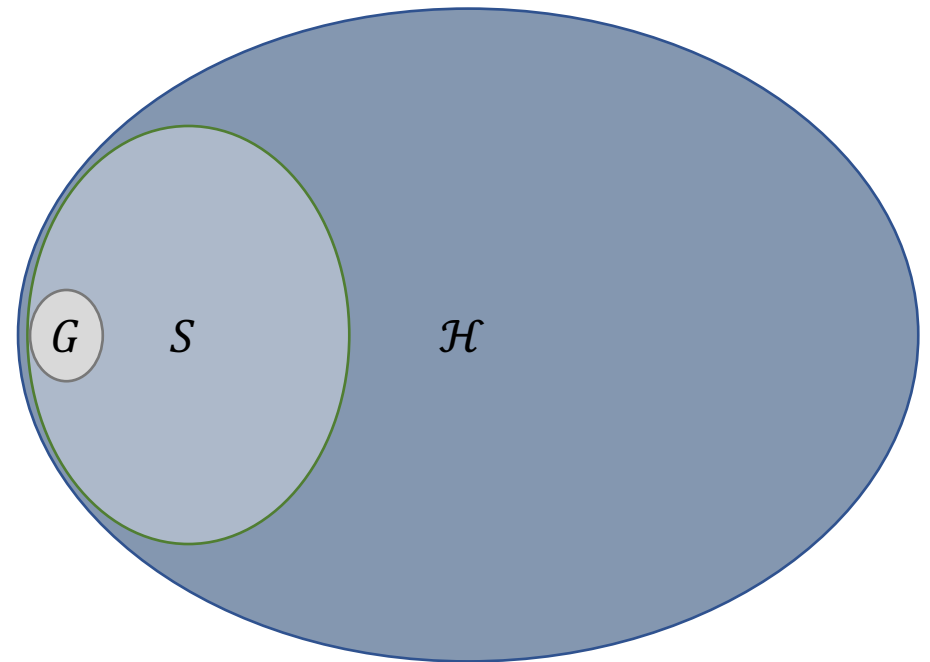
Our approach: problem-tailored ansätze

Use information from the Hamiltonian to restrict search subspace of Hilbert space

Desired features:

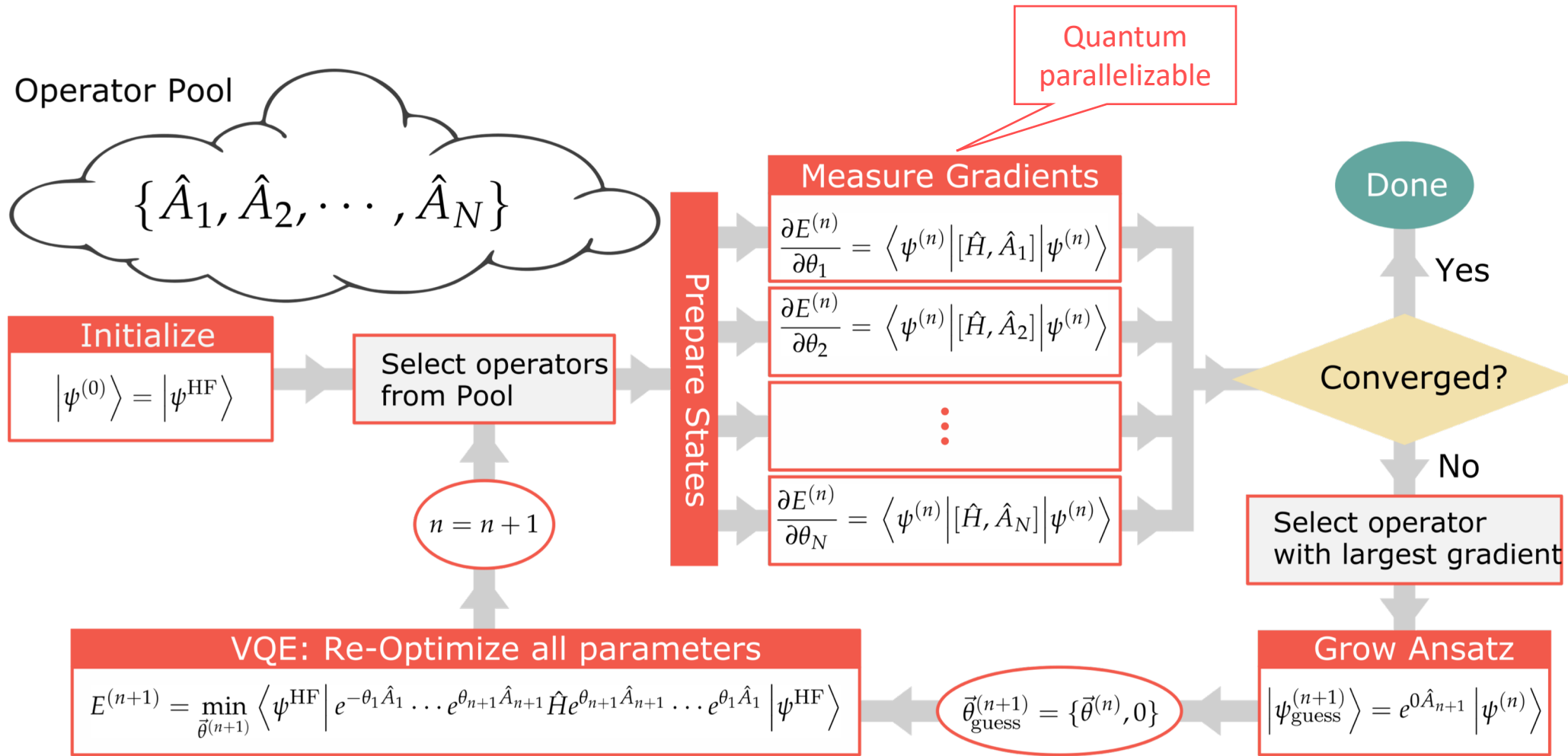
- ✓ shallow circuits
- ✓ small/minimal number of optimization parameters
- ✓ Exactness

- Symmetry enforcing circuits
- ADAPT-VQE, qubit-ADAPT-VQE

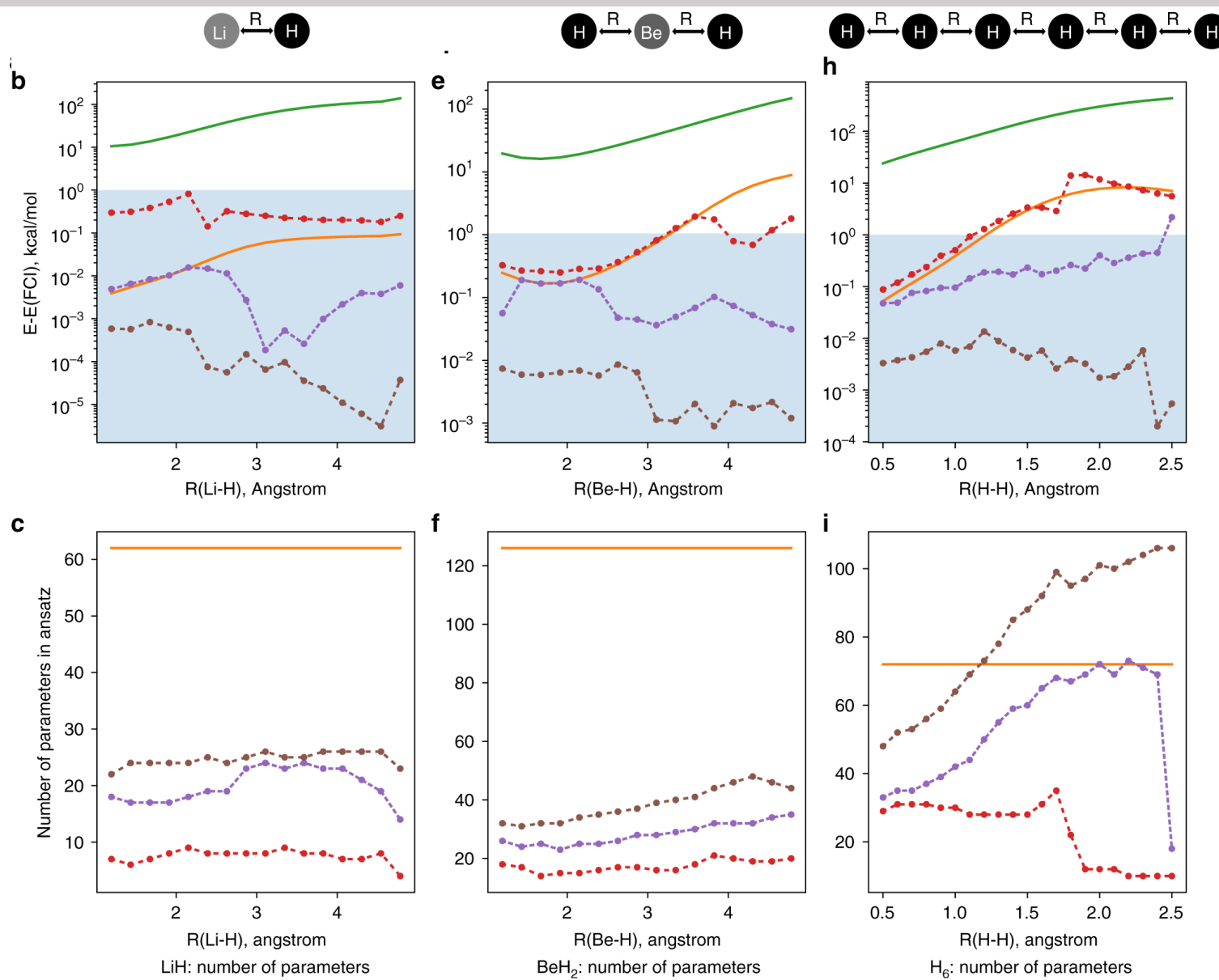


- Adaptive, Problem-tailored (ADAPT)-VQE: the first dynamically created ansatz
- Start from a simple/short-depth ansatz (e.g., Hartree-Fock)
- Use measurements on the quantum processor to determine how to grow the ansatz further
- The measurements depend on the Hamiltonian → problem-tailored ansatz

ADAPT-VQE workflow



fermionic ADAPT-VQE—results

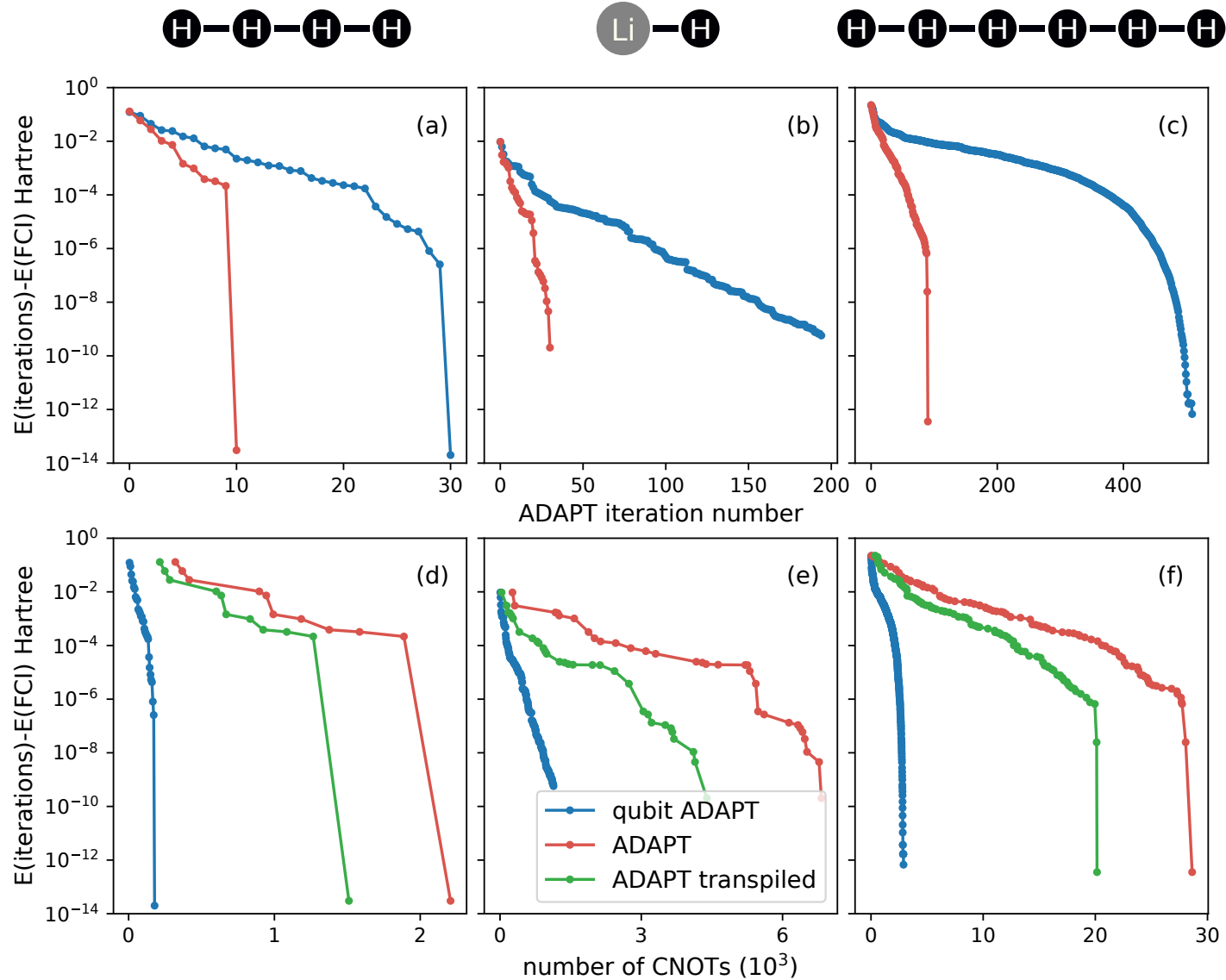


Hardware-efficient pool

$\{e^{i\theta_j P_j}\}$, where P_j is a

Pauli string with up to 4 Paulis

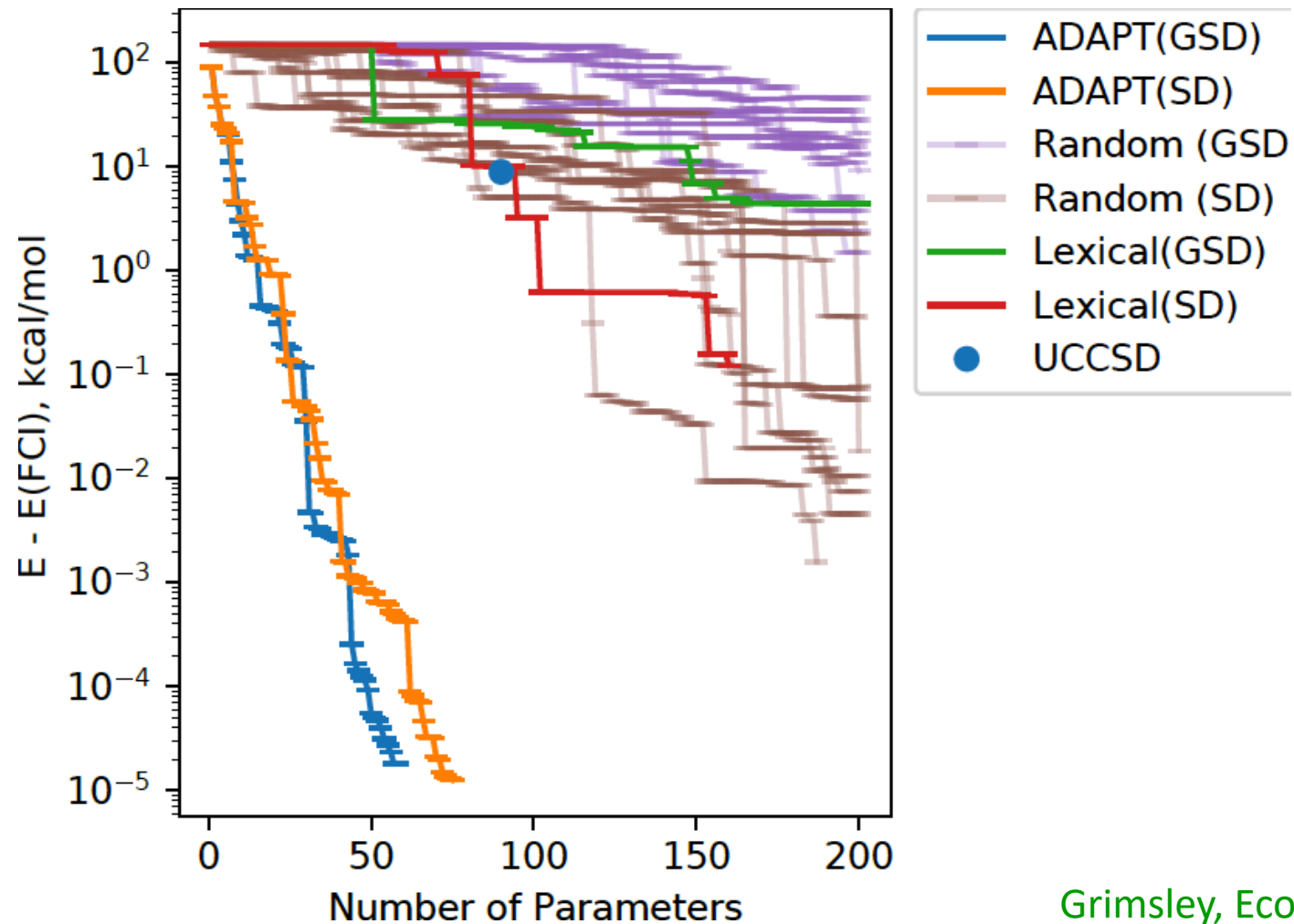
Qubit ADAPT-VQE—results



- 8, 12, 12 qubits respectively
- bond distances 1.5, 2, 1.5 Å

Tang et al,
PRX Quantum 2,
020310 (2021)

Comparing ADAPT to other operator orderings

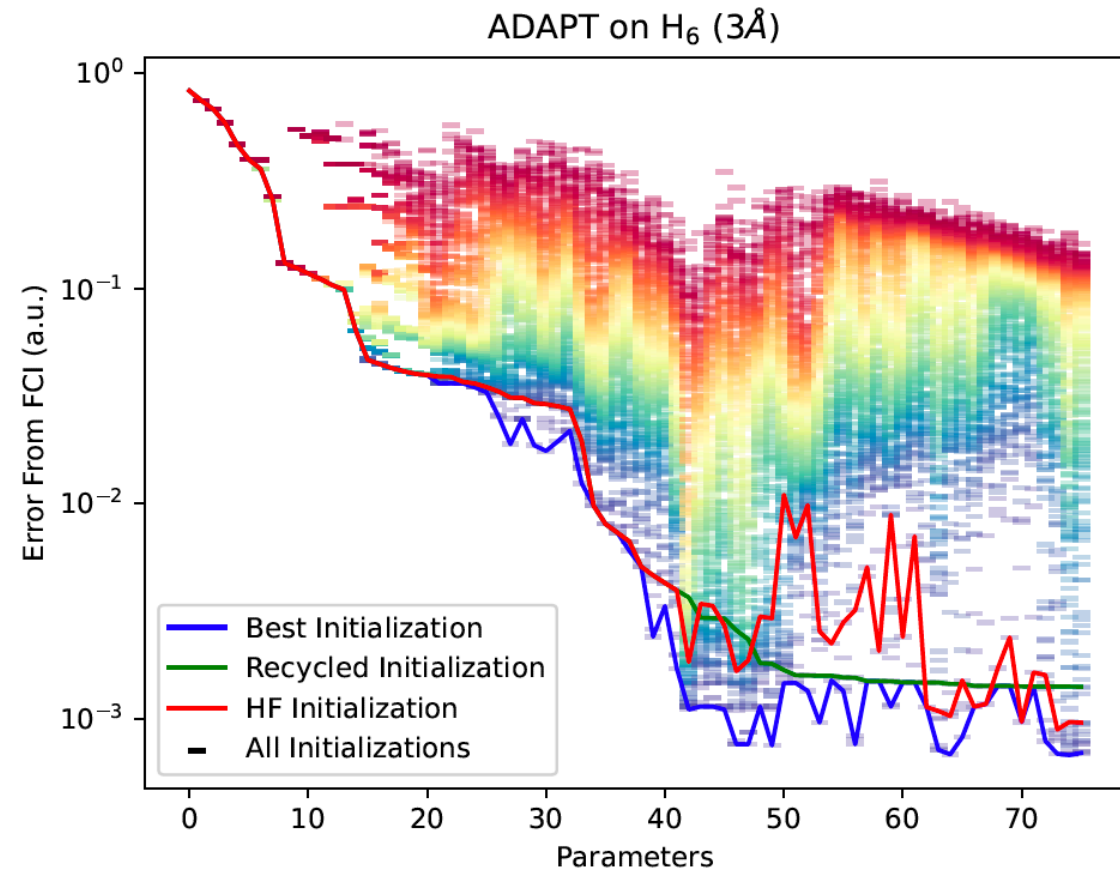


BeH_2
bond distance 2.39 Å

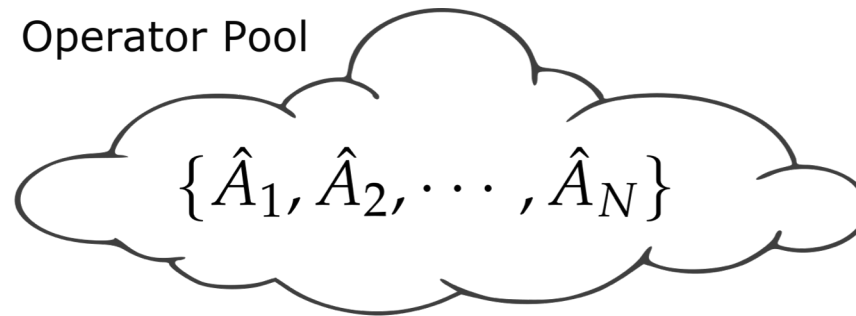
Grimsley, Economou, Barnes, Mayhall,
Nat. Commun. **10**, 3007 (2019)

Trainability of ADAPT-VQE

- ADAPT produces compact, problem-tailored ansätze
- Shallow circuit \rightarrow the landscape is generally too rugged
- Trainability?
- ADAPT avoids the issues associated with trainability by “burrowing”
- ADAPT also avoids barren plateaus because gradient is guaranteed to be large in one direction



How should the operator pool be chosen?



- We can choose it according to hardware constraints
- What are the right operators, and how many do we need?

Minimal complete pool (MCP): smallest sized complete pool

The minimal size of complete pools is linear in the nr of qubits: $2n-2$

Example of min complete pool
“G pool”

$$\left\{ \begin{array}{l} G_1 = ZYII \dots I, \quad G_2 = IZYII \dots I, \\ G_3 = IIZYII \dots I, \quad \dots, \quad G_{n-2} = II \dots IZYI, \quad G_{n-1} = II \dots IZY, \\ G_n = YII \dots I, \quad G_{n+1} = IYII \dots I, \\ G_{n+2} = IYYII \dots I, \quad \dots, \quad G_{2n-3} = II \dots IYII, \quad G_{2n-2} = II \dots IYI \end{array} \right.$$

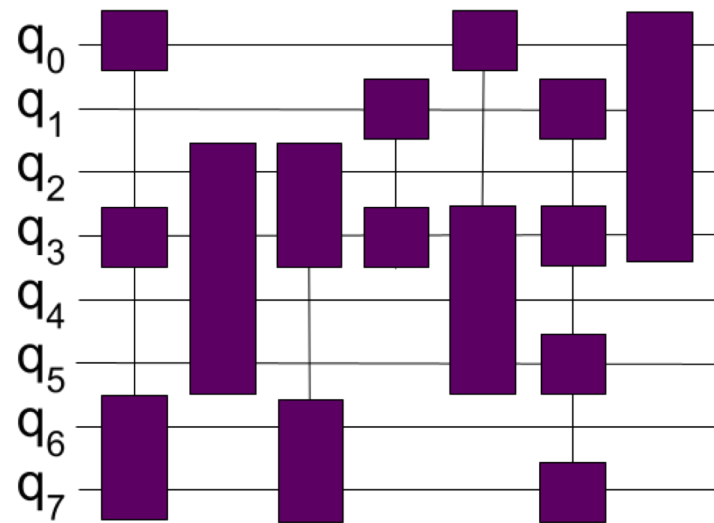
- **Proof that G is complete**
- **Proof that $2n-2$ is the minimal size of a complete pool**
- **Three criteria for identifying MCPs**
- **Incorporating symmetries into MCPs**

TETRIS-ADAPT-VQE: concept

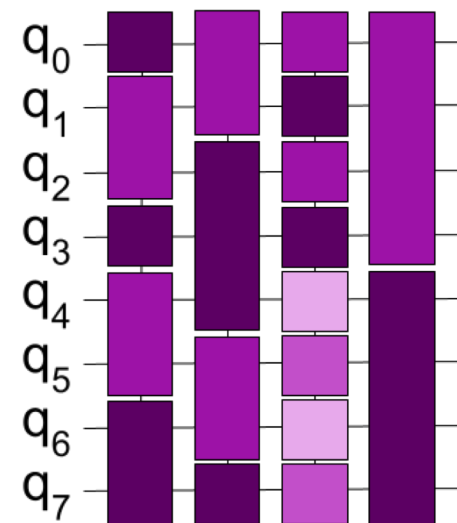
Tiling Efficient Trial circuits with Rotations Implemented Simultaneously

Instead of one-at-a-time, add multiple operators at each step according to:

- Gradient magnitude
- \mathcal{N} th operator acting on different set of qubits from $(\mathcal{N} - j)$ th

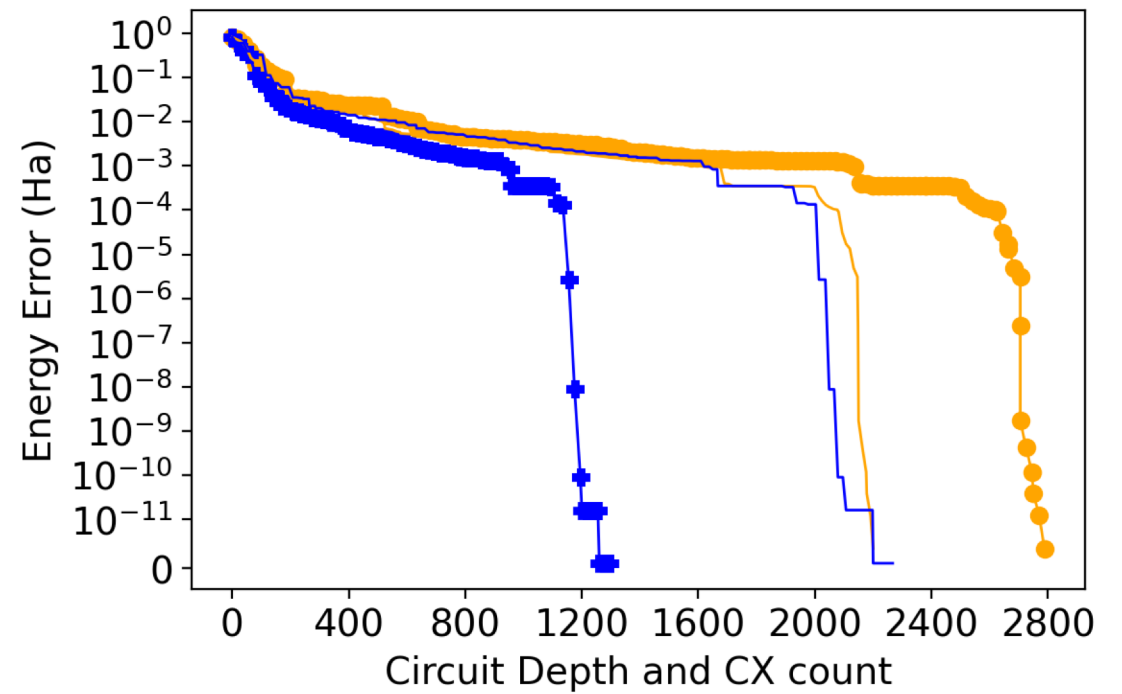
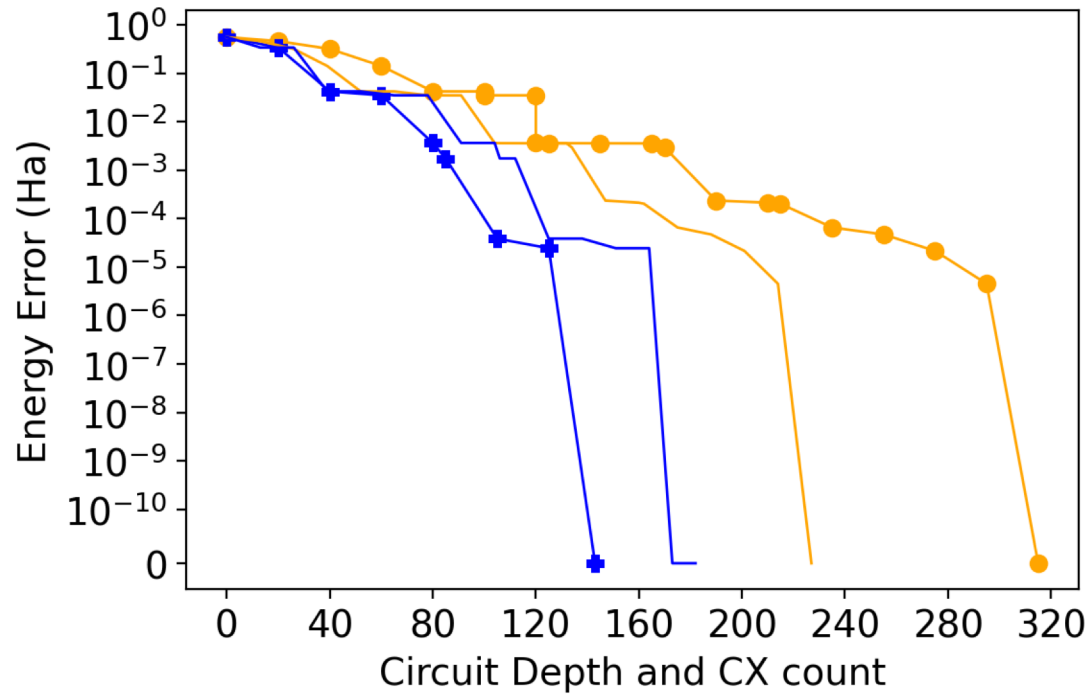
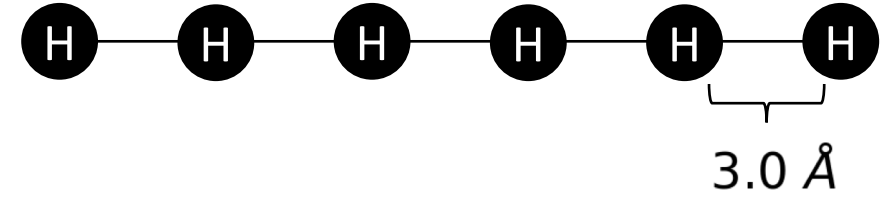
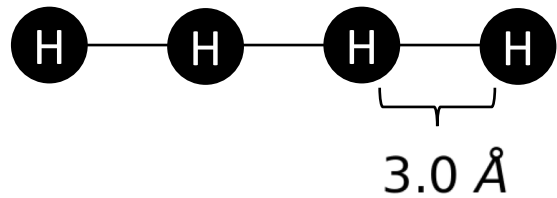


ADAPT-VQE



TETRIS-ADAPT-VQE

TETRIS-ADAPT-VQE: results



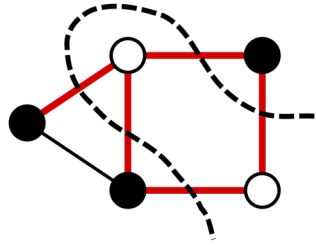
Blue: TETRIS-ADAPT

Orange: standard ADAPT

Anastasiou, Chen, et al, arXiv:2209.10562

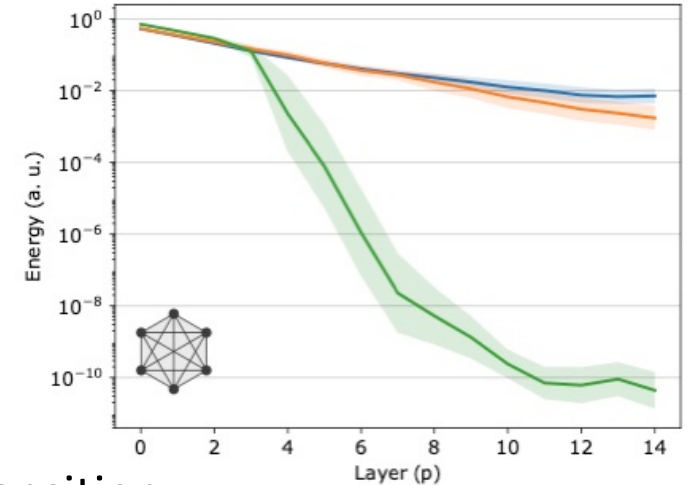
Other applications of ADAPT-VQE

- Optimization: ADAPT-QAOA, where we use ADAPT to determine mixers



Zhu et al, PRR 4, 033029 (2022)

Chen et al, arxiv:2205.12283



- Nuclear physics: LMG ('Lipkin' model), where ADAPT finds g.s. across phase transition

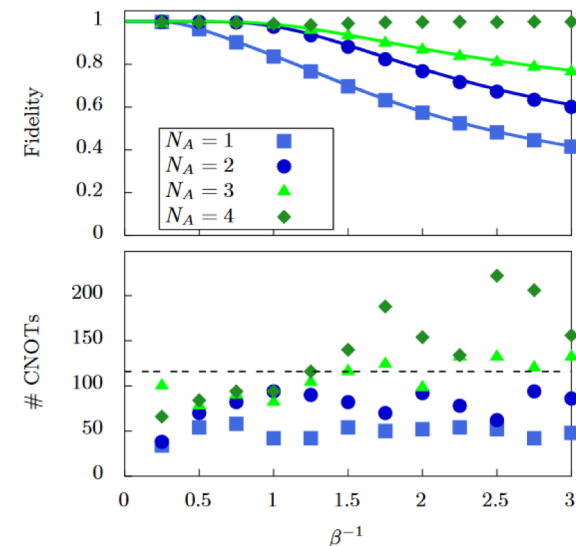
Romero et al, Phys. Rev. C 105, 064317 (2022)

- Spin Hamiltonians with lattice structure, small instances and scale up through 'tiling'

Van Dyke et al, 2206.14215

- Gibbs state preparation: new, easier to measure objective function; ADAPT strategy reduces resource requirements

Warren et al, arXiv: 2203.12757



Non-variational routes to quantum advantage?

Are there problems for which we know a lot about the solutions, but not everything?

Can we use what we know about the solutions to design efficient algorithms to figure out the parts we don't know?

Bethe Ansatz



[Wikipedia]

H. Bethe, “Zur Theorie der Metalle” *Z. Physik* **71**, 205 (1931).

Solved Heisenberg chain in 1D



Began a new subfield of mathematical physics

XXZ, Hubbard, Lieb-Liniger, Kondo, Richardson-Gaudin,...

Exact solutions of interacting many-body models

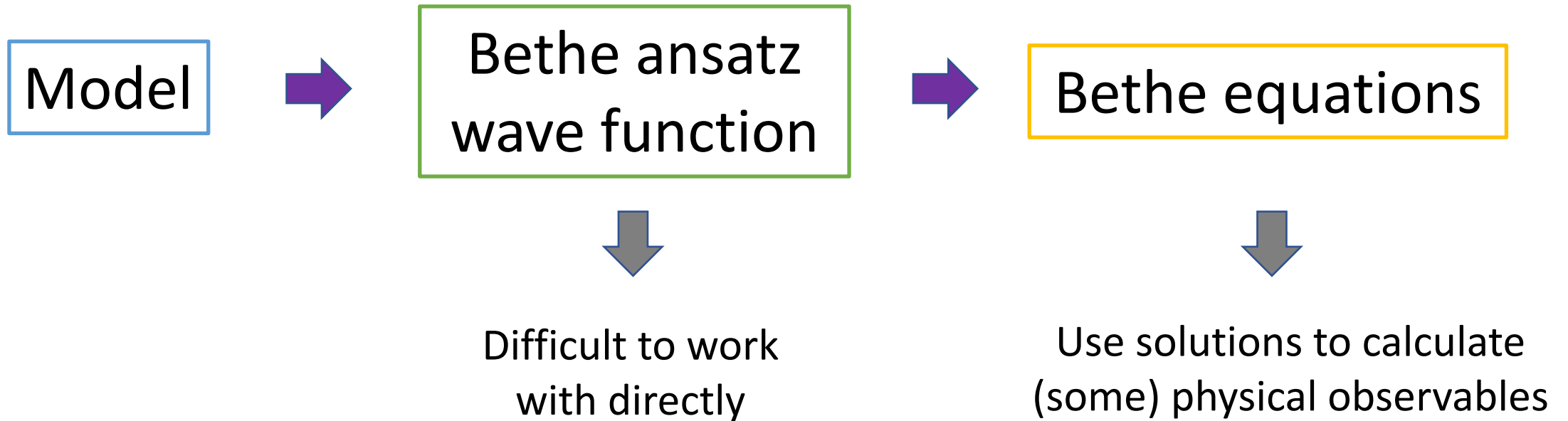
Korepin *et al.*, *Quantum Inverse Scattering Method and Correlation Functions* (1993)

Takahashi, *Thermodynamics of One-Dimensional Solvable Models* (1999) ²³

Essler *et al.*, *The One-Dimensional Hubbard Model* (2005)

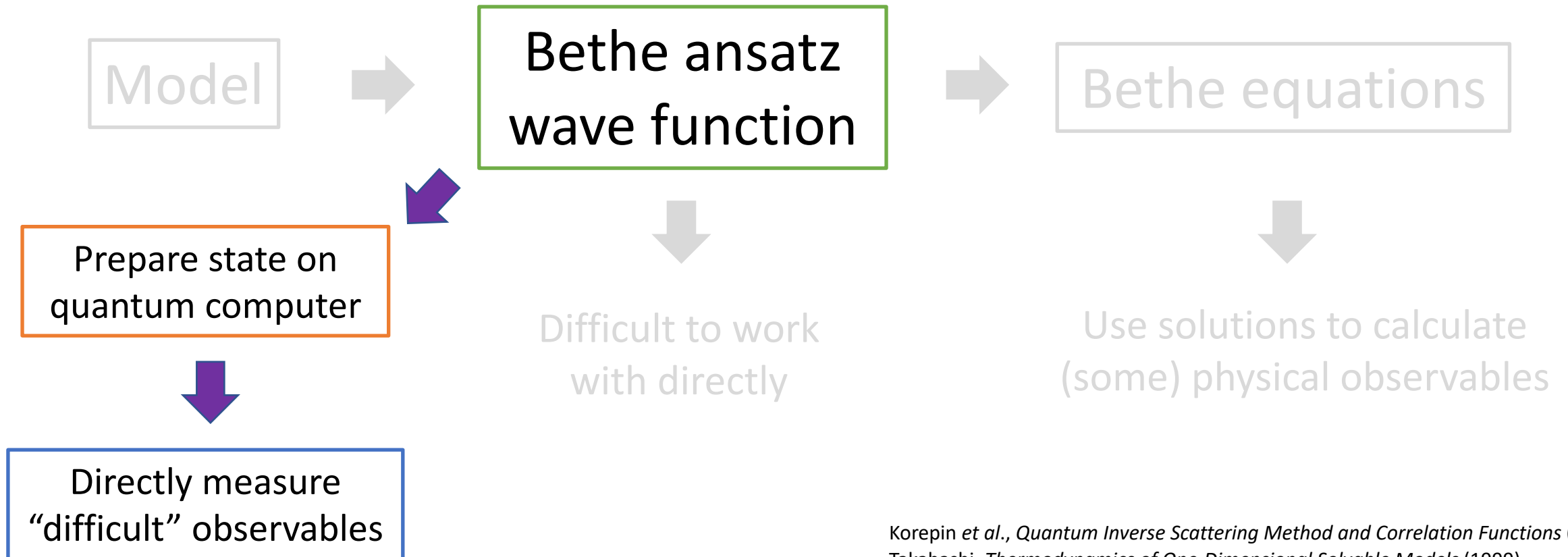
Quantum Advantage?

exact solution \neq complete knowledge



Quantum Advantage?

exact solution \neq complete knowledge



Bethe Ansatz: XXZ chain

XXZ spin chain:

(anisotropic Heisenberg model)

$$H_{XXZ} = J \sum_{j=1}^L \left[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z \right]$$

w/ periodic
boundary conditions

$$[H_{XXZ}, S_{tot}^z] = 0$$




Consider states with fixed number of down spins

Bethe Ansatz: XXZ chain

Solution: $|\psi_B\rangle = \sum_{x_1 < x_2 < \dots} \psi(x_1, x_2, \dots) |\uparrow \cdots \downarrow_{x_2} \cdots \uparrow \cdots \downarrow_{x_1} \cdots \uparrow\rangle$

$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

Permutations of
down spin positions



$$A_P = e^{-i\Theta_{\alpha,\beta}} e^{-i\Theta_{\gamma,\delta}} \dots e^{-i\Theta_{\epsilon,\zeta}}$$

Phases from transpositions defining P



k_j values determined from Bethe equations:

$$Lk_i = 2\pi I_i + \sum_j \Theta(k_i, k_j)$$

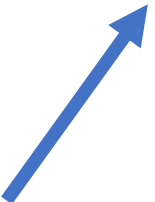
$$\begin{aligned} \frac{A_P}{A_{P'}} &= - \frac{1 + e^{i(k_{Pl} + k_{P'l})} - 2\Delta e^{ik_{Pl}}}{1 + e^{i(k_{Pl} + k_{P'l})} - 2\Delta e^{ik_{P'l}}} \\ &\equiv -e^{-i\Theta(k_{Pl}, k_{P'l})}. \end{aligned}$$

Bethe Ansatz State Preparation

Goal: Design an algorithm to prepare XXZ chain eigenstates

- Van Dyke, *et al.*, PRX Quantum 2, 040329 (2021)

$$|\psi_B\rangle = \sum_{x_1 < x_2 < \dots} \psi(x_1, x_2, \dots) |\uparrow \cdots \downarrow_{x_2} \cdots \uparrow \cdots \downarrow_{x_1} \cdots \uparrow\rangle$$


$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

Linear Combination of Unitaries

Childs & Wiebe, QIC 12, 901 (2012)
Berry *et al.*, PRL 114 090502 (2015)

Linear Combination of Unitaries

Want to implement a sum of unitary operations: $\tilde{U} = \sum_j \beta_j V_j$

Idea: execute individual terms using an ancilla register:

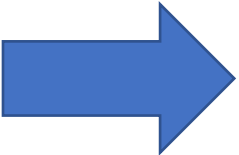
$$\text{select}(V)|j\rangle|\psi\rangle = |j\rangle V_j |\psi\rangle$$

Prepare ancilla in a superposition

$$B|0\rangle = \frac{1}{\sqrt{s}} \sum_j \sqrt{\beta_j} |j\rangle, \quad s = \sum_j \beta_j$$

Linear Combination of Unitaries

Defining $W = (B^\dagger \otimes \mathbb{1}) \text{select}(V) (B \otimes \mathbb{1})$

 $W|0\rangle|\psi\rangle = \underbrace{\frac{1}{s}|0\rangle\tilde{U}|\psi\rangle}_{\text{success}} + \sqrt{1 - \frac{1}{s^2}}|\Phi\rangle|\text{junk}\rangle$

$\langle 0|\Phi\rangle = 0$

The diagram shows a blue arrow pointing to the left-hand side of the equation. A blue bracket is placed under the term $\frac{1}{s}|0\rangle\tilde{U}|\psi\rangle$. A purple arrow points from the text $\langle 0|\Phi\rangle = 0$ to the term $|\Phi\rangle|\text{junk}\rangle$ in the equation.

If measure $|0\rangle$, then success

Bethe Ansatz Algorithm

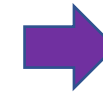
Highlight two aspects:

$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

1. Implementing the A_p factors

of controlled phases:

~~$M!$~~
(naïve)



$O(M^3)$
(our method)

2. Implementing the e^{ikx} factors

of controlled phases:

~~$M! \binom{L}{M}$~~
(naïve)



$O(M^2 L)$
(our method)

Bethe State Preparation

$$|\psi_B\rangle = \sum_{x_1 < x_2 < \dots} \psi(x_1, x_2, \dots) |\uparrow \dots \downarrow_{x_2} \dots \uparrow \dots \downarrow_{x_1} \dots \uparrow\rangle$$

$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

Full Quantum Register:

$$|\Psi\rangle = |w\rangle |\dots\rangle_f |\dots\rangle_p |\dots\rangle_s$$

work qubit

“faucet” ancillas
[M qubits]

permutation label
[M² qubits]

system subregister
[L qubits]

Quantum Algorithm

Bethe state preparation algorithm:

$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

1. Prepare the Dicke state $|D_{L,M}\rangle$
2. Construct the permutation label while generating the phases A_P
3. Apply site-dependent phases using the “faucet” method
4. Invert the permutation label (without phases)
5. Measure the permutation label, with success on finding $|00 \dots 0\rangle$

Step 1: Dicke States

Dicke state $|D_{L,M}\rangle$ = Equal superposition of all states on L sites with M down spins

$$|D_{4,2}\rangle = \frac{1}{\sqrt{6}} \left[|\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle \right]$$

Dicke state preparation:

- Bärtschi & Eidenbenz (2019): deterministic algorithm, $O(LM)$
- Mukherjee et al. (2020): improved gate count

Step 2: Permutation Labels

$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

Need to sum on permutations

How to label the different permutations?

$M=3$:

Group Elements		
()		
(1,2)		
(2,3)		
(1,3)		
(1,2,3)		
(1,3,2)		

Step 2: Permutation Labels

$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

Need to sum on permutations

How to label the different permutations?

$M=3$:

Group Elements	Simple Counter	
()	1>	
(1,2)	2>	
(2,3)	3>	
(1,3)	4>	
(1,2,3)	5>	
(1,3,2)	6>	

Step 2: Permutation Labels

$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

Need to sum on permutations

How to label the different permutations?

$M=3$:

Group Elements	Simple Counter	Explicit Representation
()	1>	1> 2> 3>
(1,2)	2>	2> 1> 3>
(2,3)	3>	1> 3> 2>
(1,3)	4>	3> 2> 1>
(1,2,3)	5>	3> 1> 2>
(1,3,2)	6>	2> 3> 1>

Step 2: Permutation Labels

Represent each down spin using a one-hot encoding

$$1: |001\rangle \equiv |1\rangle$$

$$2: |010\rangle \equiv |2\rangle$$

$$3: |100\rangle \equiv |3\rangle$$

Need three “slots” to express the action of a given permutation on the down spin labels

$$|\dots\rangle |\dots\rangle |\dots\rangle$$

Implement permutations on the labels using “partial SWAP” operations

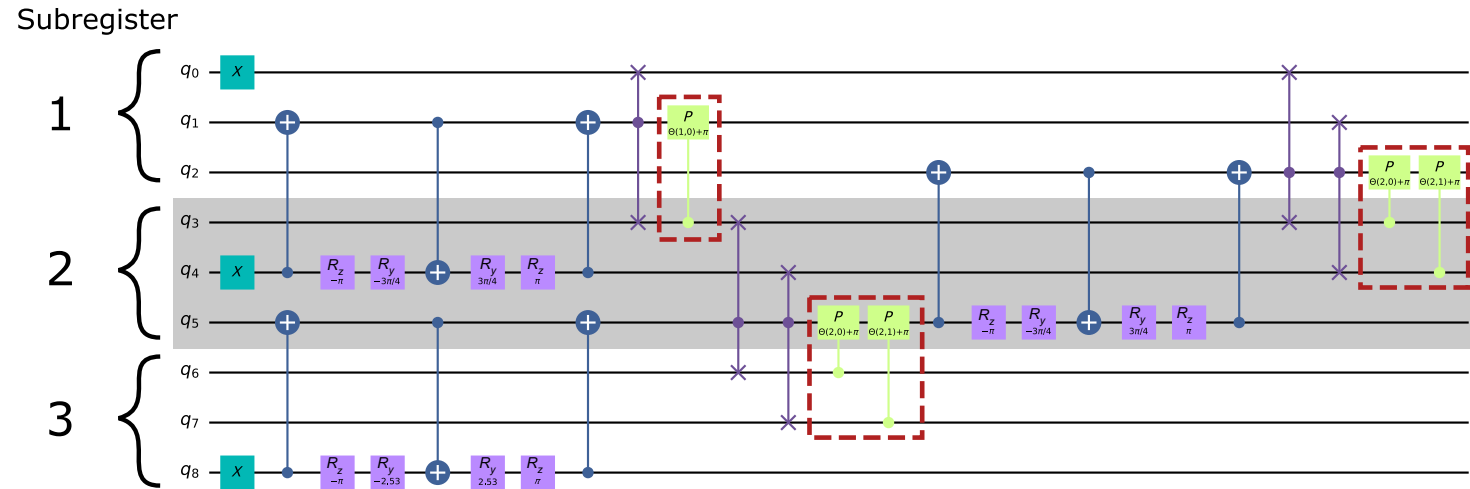
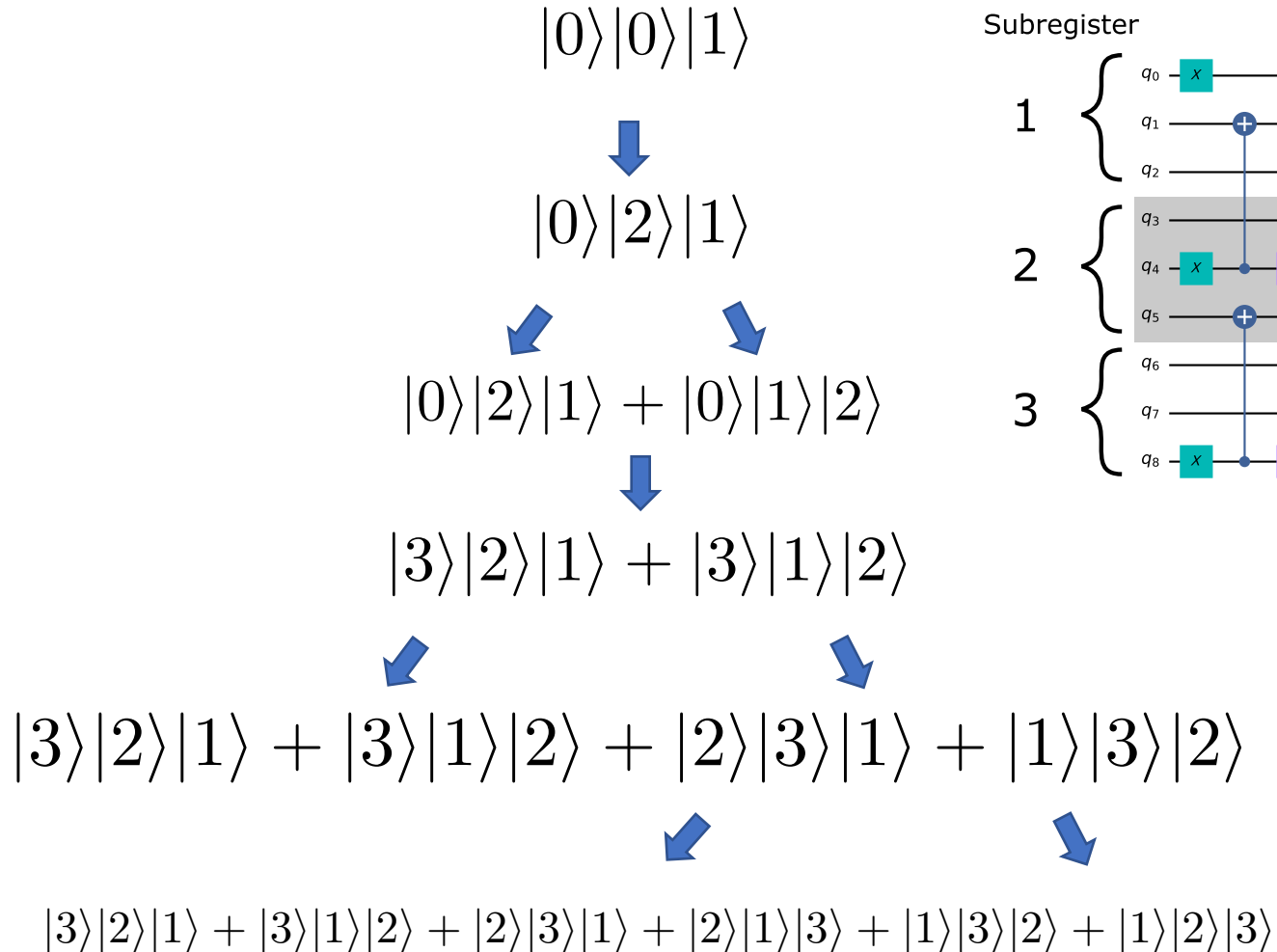
$$A(\theta, \phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & e^{i\phi} \sin(\theta) & 0 \\ 0 & e^{-i\phi} \sin(\theta) & -\cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Produces a superposition of “SWAP” + “no SWAP”

$$|10\rangle \rightarrow -\cos(\theta)|10\rangle + e^{i\phi} \sin(\theta)|01\rangle$$

Step 2: Permutation Labels

Construct the label iteratively by SWAPs on the different slots

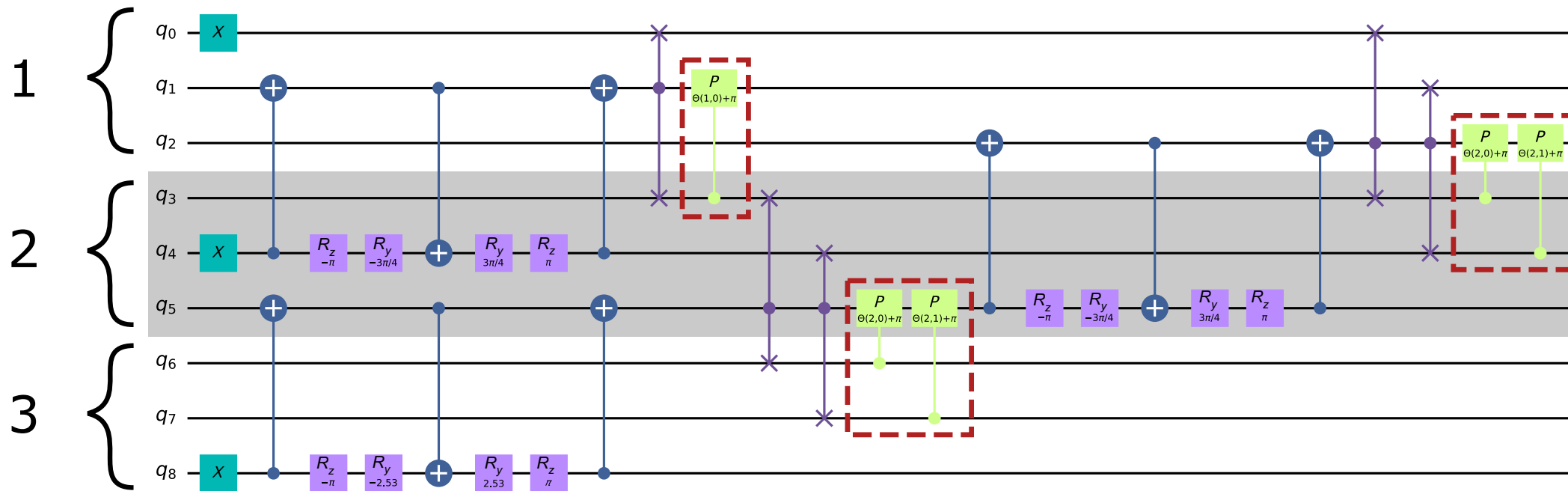


Step 2: Permutation Labels

$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

Generate the $A_P = (-1)^s e^{-i\Theta_{\alpha\beta}} \dots e^{-i\Theta_{\gamma\delta}}$ on the fly while swapping labels

Subregister



Step 3: Site-dependent Phases

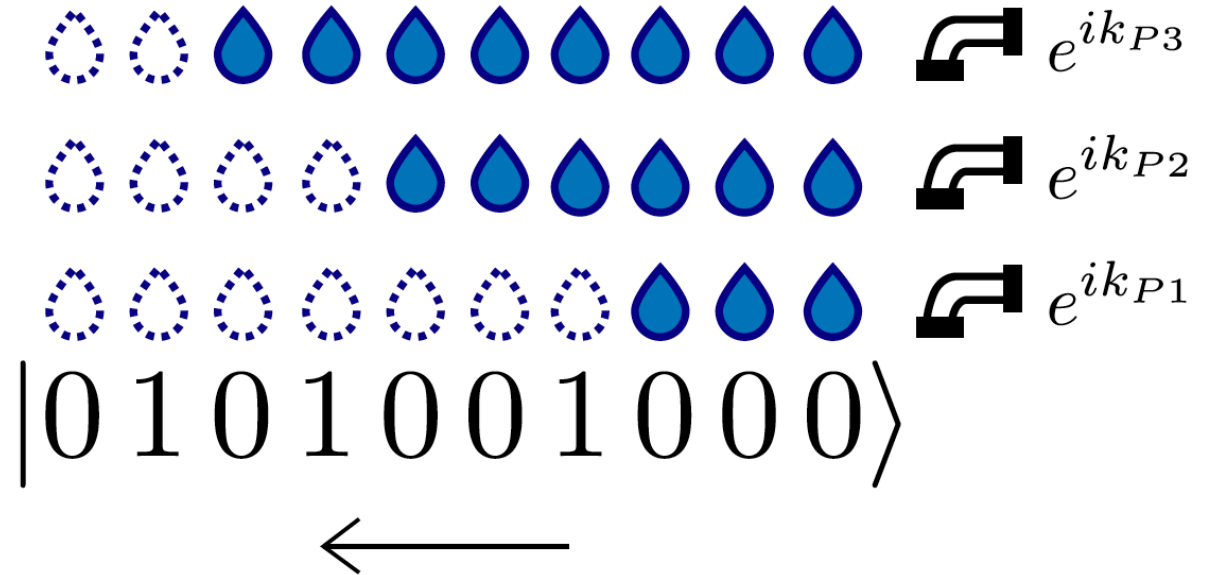
$$\psi(x_1, \dots, x_M) = \sum_P A_P \exp \left[i \sum_{j=1}^M k_{Pj} x_j \right]$$

“Faucet method”

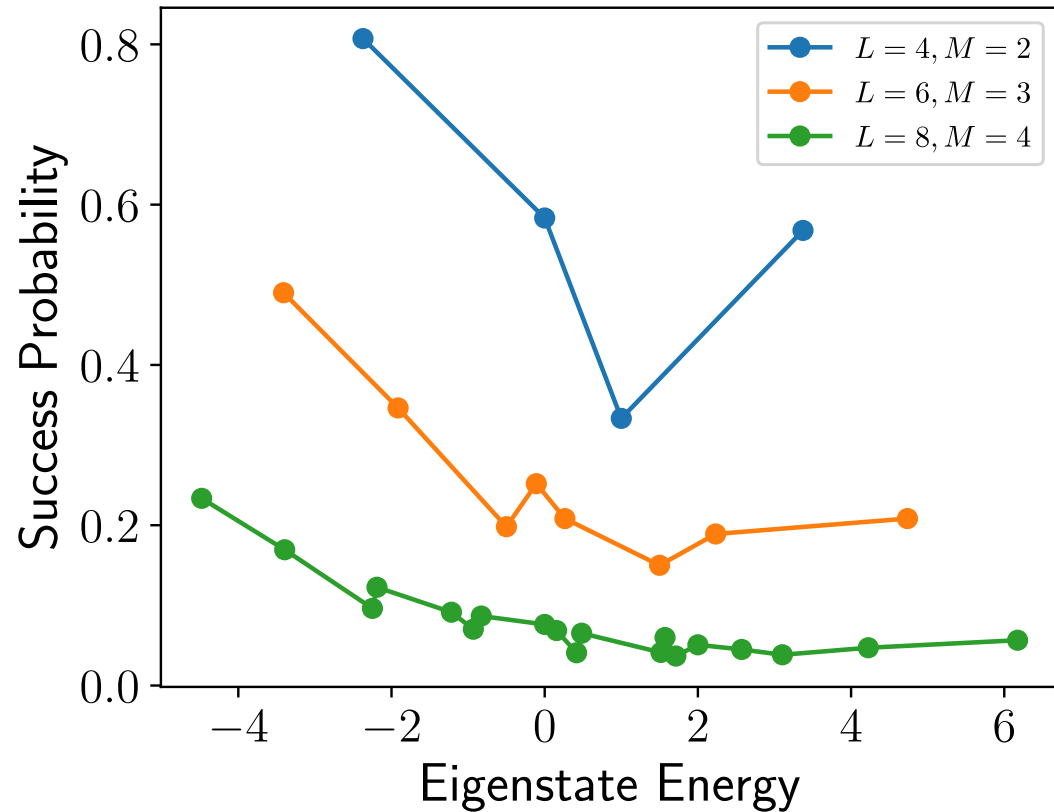
x_j = position of down spin
(integer)

apply $e^{ik_{Pj}}$ repeatedly, site by site

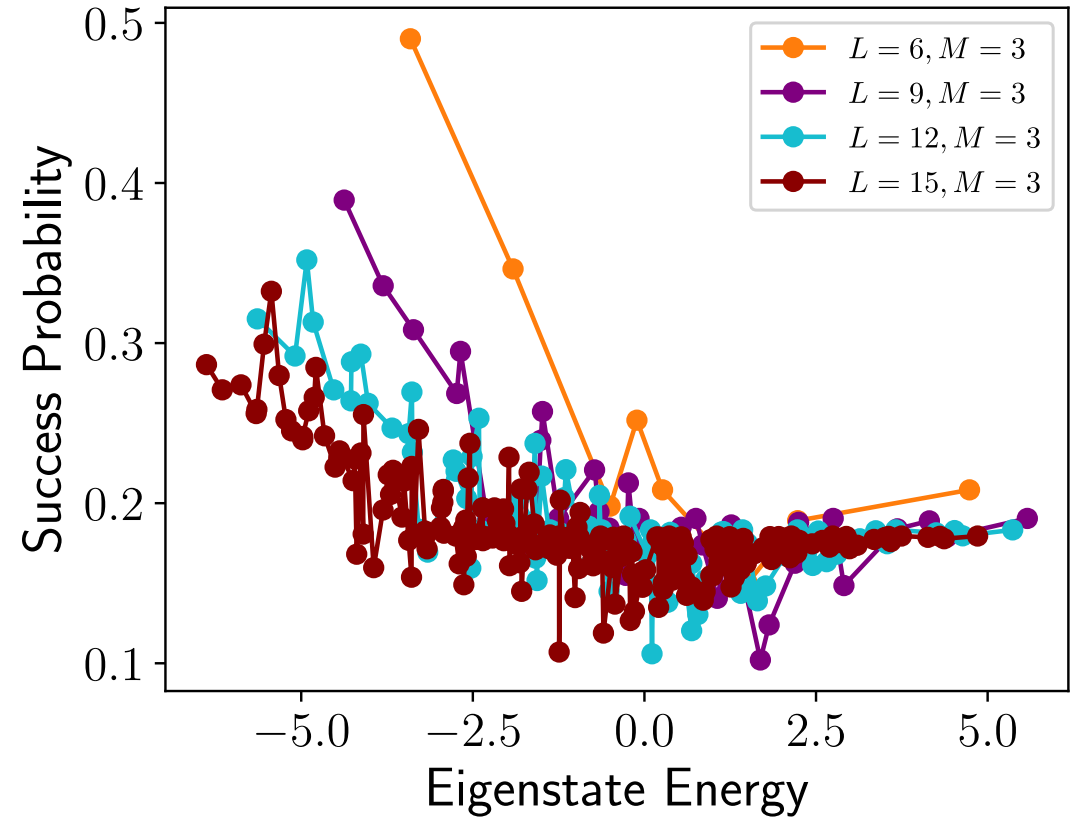
‘turn off’ the phase gate when you reach a down spin



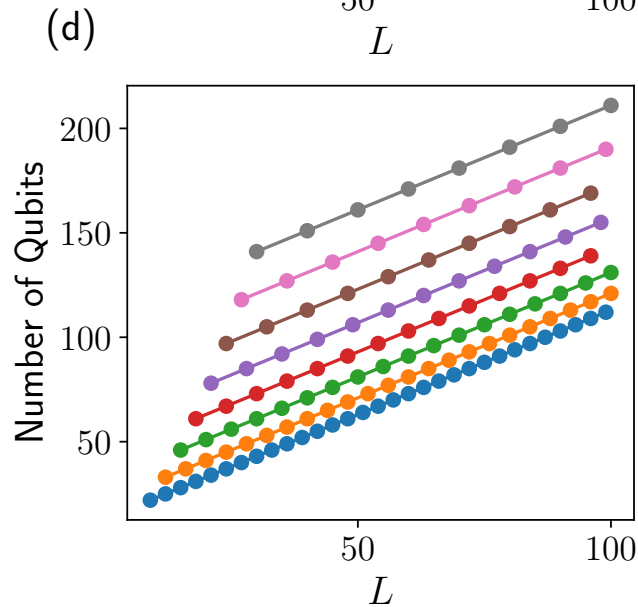
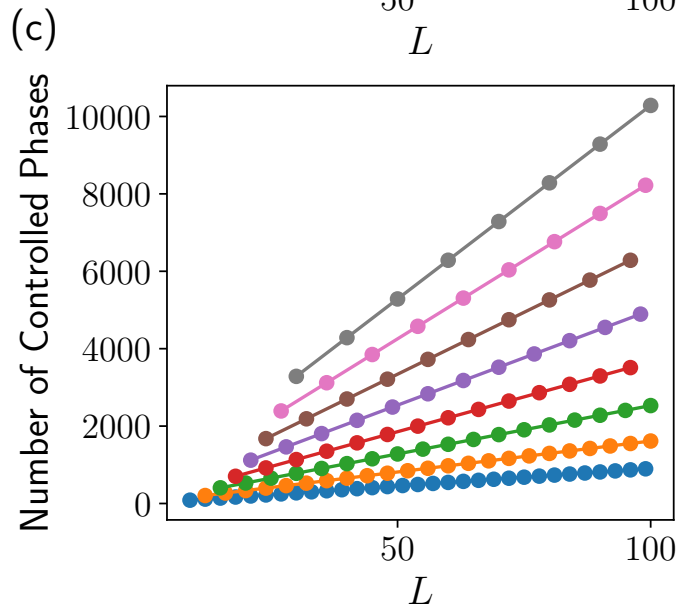
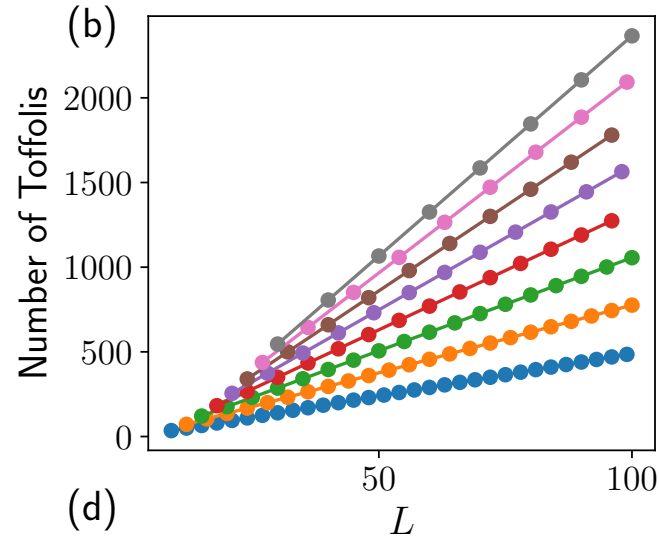
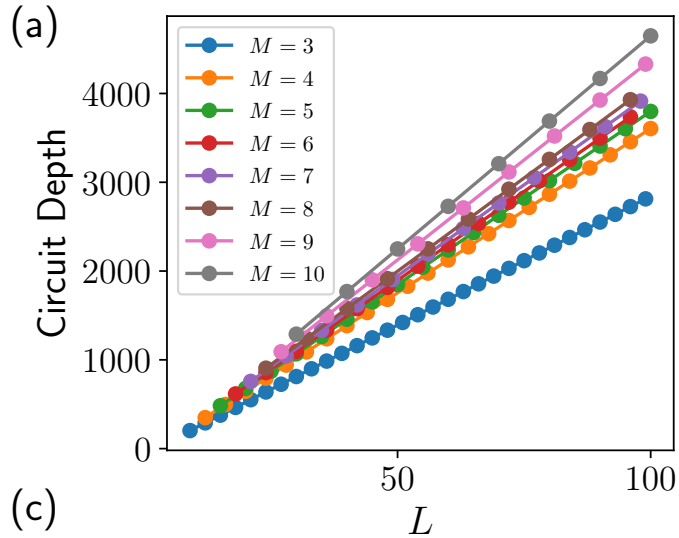
Numerics: Success Probability



$$J = 2, \Delta = -1/2$$



Numerics: Resources



$L=100, M=5$:

≈ 2000 Toffolis

≈ 2000 Controlled phases

≈ 130 logical qubits

≈ 120 repetitions for success

States live in a $\binom{100}{5} \approx 7.5 \times 10^7$
dimensional subspace

T gate estimate $\approx 4.1 \times 10^6$
(with amplitude amplification)

Amplitude amplification

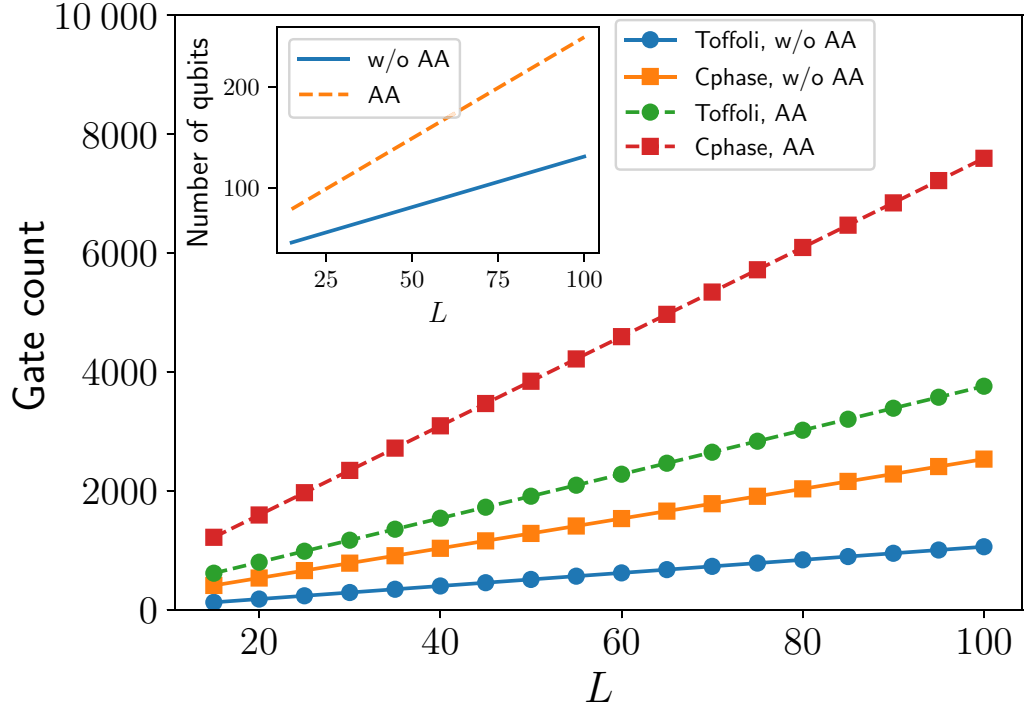
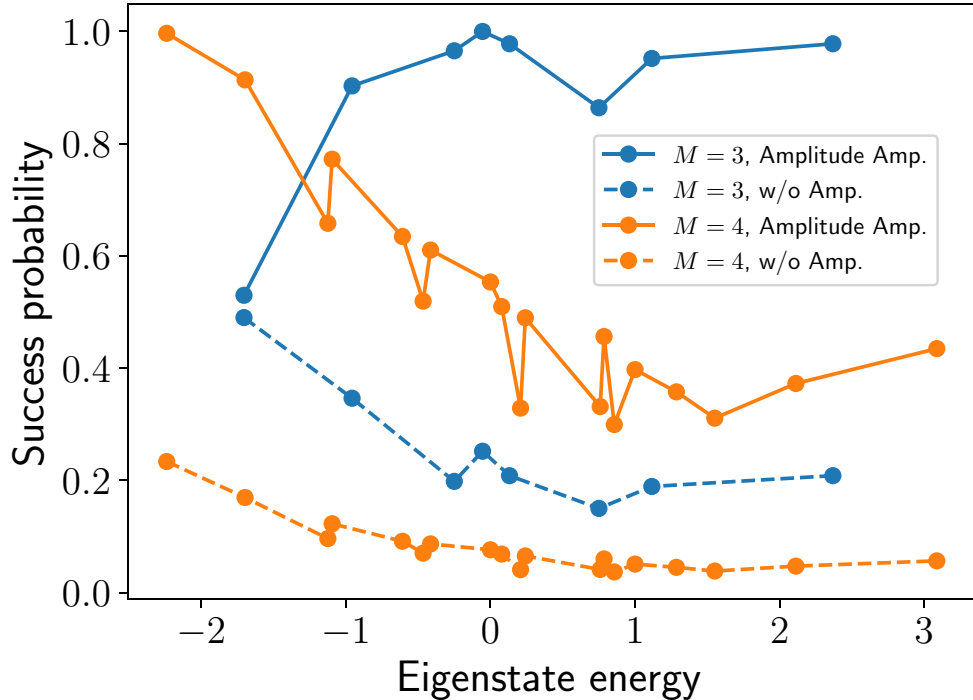
Apply to pre-measurement state:

$$Q = -\mathcal{B}S_0\mathcal{B}^{-1}S_B$$

Bethe circuit

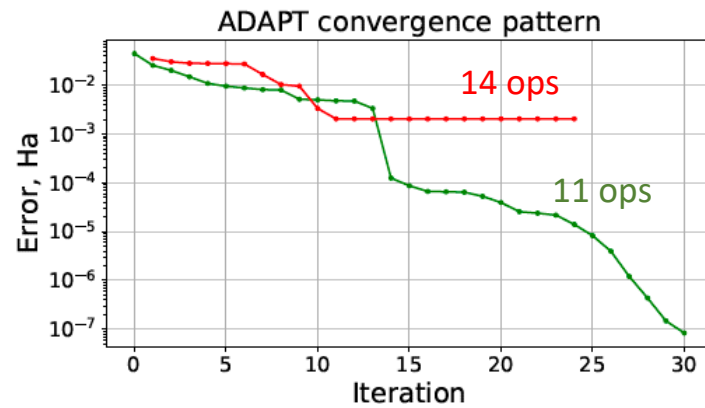
Changes sign of $|000\dots 0\rangle$ on permutation label

Changes sign of $|000\dots 0\rangle$ on permutation label



Conclusions

ADAPT-VQE

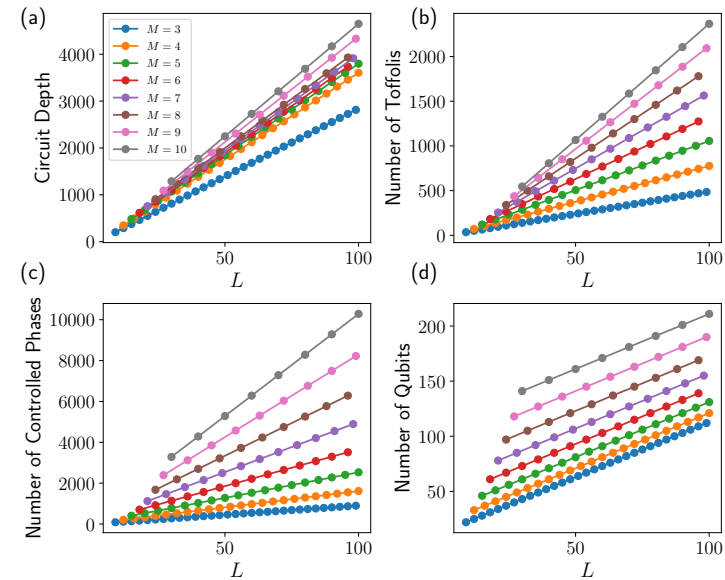


Grimsley et al,
Nat. Commun. **10**, 3007 (2019)

Tang et al, PRX Quantum **2**,
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Shkolnikov, Mayhall, Economou,
Barnes, arXiv:2109.05340

Bethe ansatz preparation algorithm

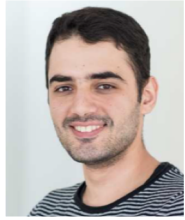


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040329 (2021)

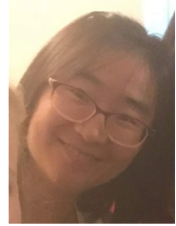
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Acknowledgements

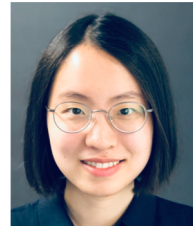
Group:



Vlad Shkolnikov



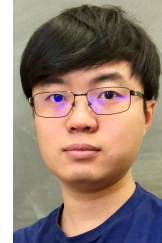
Fei Zhuang



Yanzhu Chen



Zahra Raissi



Bikun Li



Kyle Connelly



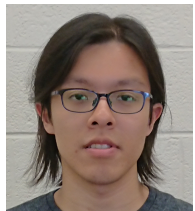
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Nooshin Estakhri



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Ada Warren



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Virginia Tech



Harper Grimsley
Virginia Tech

Variational Gibbs state preparation

Instead of preparing energy eigenstates, we can try to use variational methods to prepare physical systems at finite temperature $\rho_G = \frac{1}{Z(\beta)} e^{-\beta H}$

- Desired quantum state is no longer pure \rightarrow need extra (ancilla) qubits to entangle with
- No longer minimizes energy, but Gibbs free energy (difficult to measure)

$$F(\theta) = E(\theta) - T S(\theta) = \text{Tr}(\rho(\theta) H) + k_B T \text{Tr}(\rho(\theta) \ln \rho(\theta))$$

- With suitable objective function, can use ADAPT to prepare states efficiently

$$C(\rho(\vec{\theta})) = -\text{Tr}(\rho_G(T)\rho(\vec{\theta})) + \frac{1}{2}\text{Tr}(\rho(\vec{\theta})^2)$$

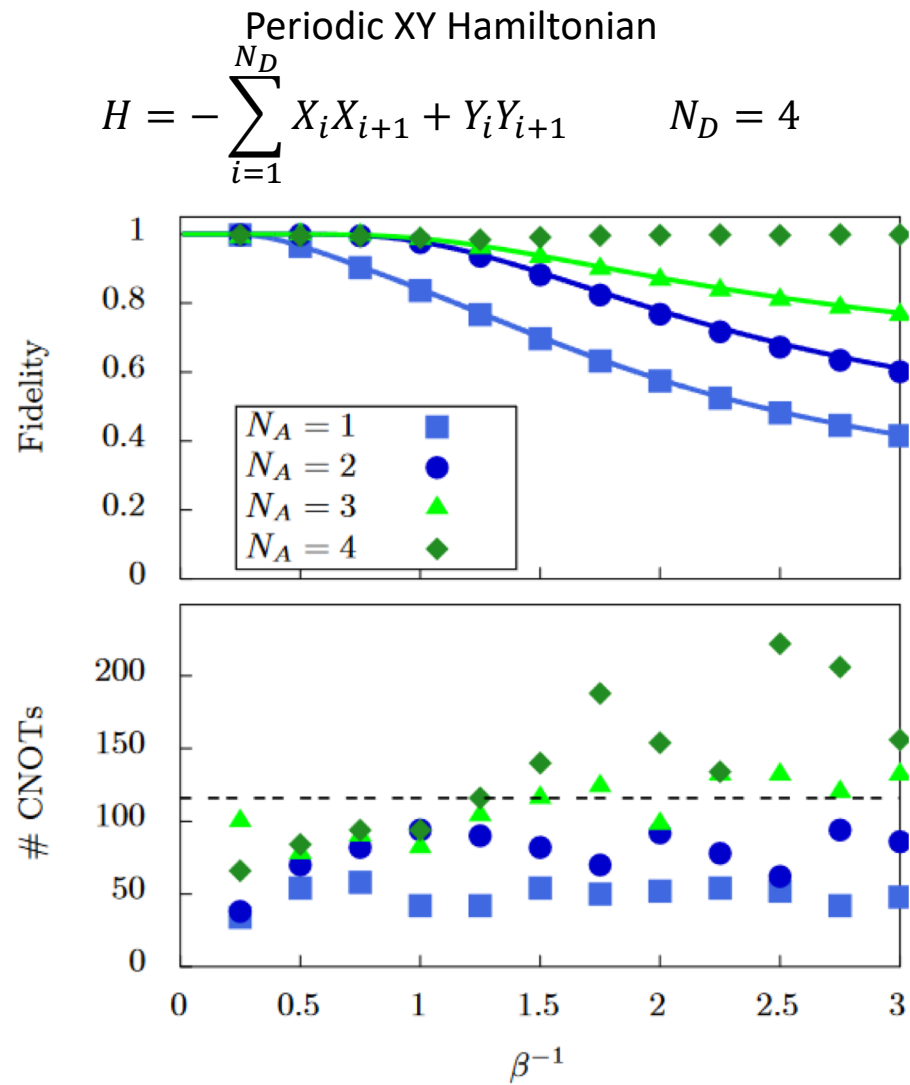
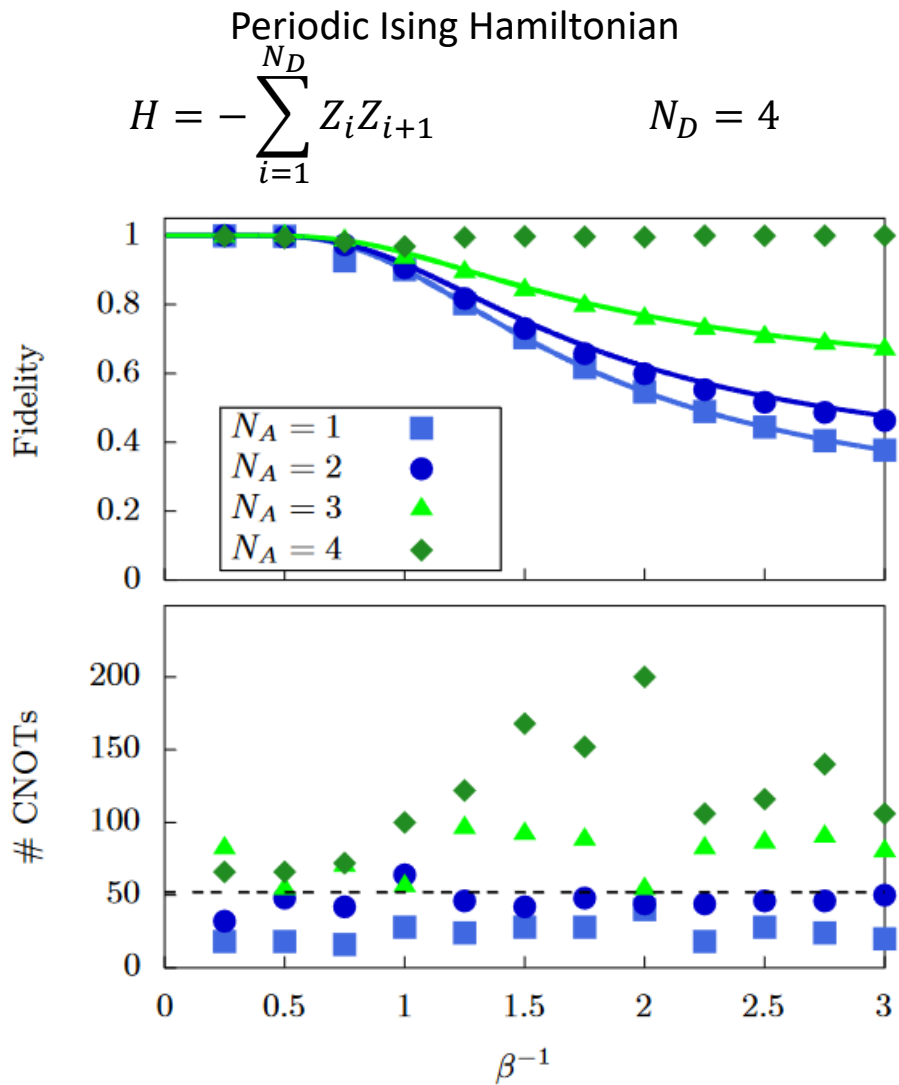
Wu and Hsieh. PRL **123**, 220502 (2019)

Chowdhury, Low, and Wiebe. arXiv:2002:00055 (2020)

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Warren, Zhu, Mayhall, Barnes, Economou. arXiv:2203.12757

ADAPT-VQE-Gibbs



L=4, M=2

