# Experimental estimation of ground state energies on quantum computers

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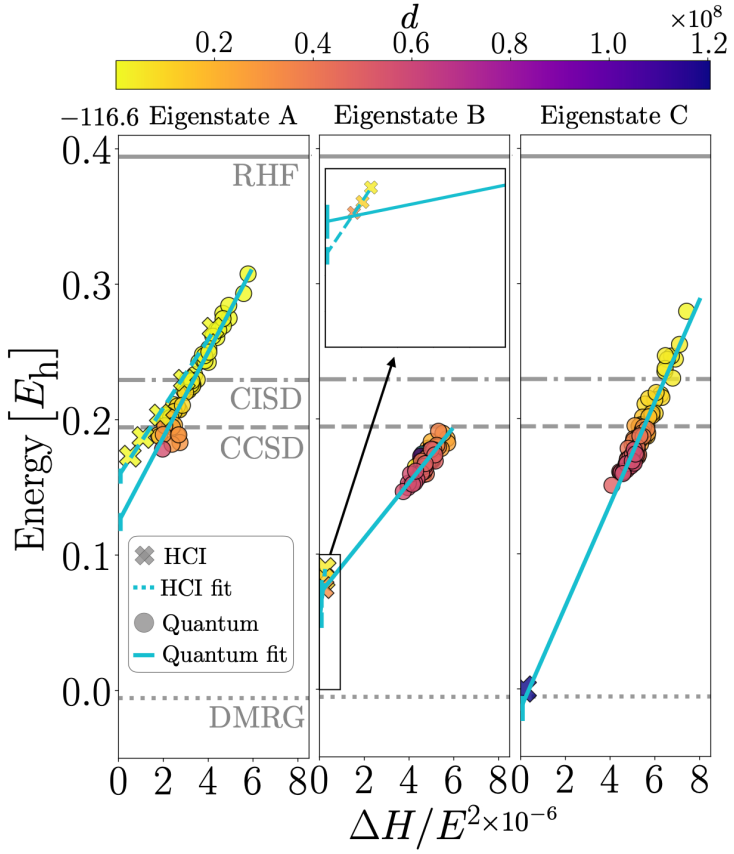


# Outline

Time permitting, I will discuss results of two recent large-scale ground state energy simulation experiments from IBM Quantum.

1. Many-body experiment using Krylov quantum diagonalization (arxiv:2407.14431)

2. Chemistry experiment using sample-based quantum diagonalization (arxiv:2405.05068)

Please interrupt with questions!


arXiv > quant-ph > arXiv:2407.14431

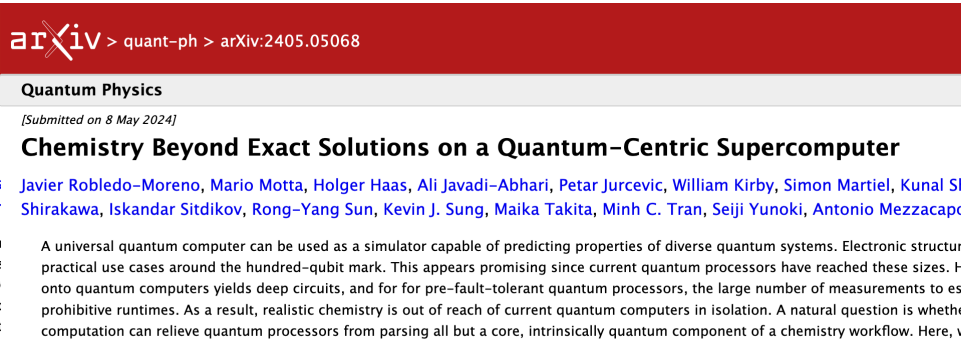
Quantum Physics

[Submitted on 19 Jul 2024 (v1), last revised 3 Oct 2024 (this version, v3)]

**Diagonalization of large many-body Hamiltonians on a quantum processor**

Nobuyuki Yoshioka, Mirko Amico, William Kirby, Petar Jurcevic, Arkopal Dutt, Bryce Fuller, Shelly Garion, Holger Haas, Ikko Hi
Ritajit Majumdar, Zlatko Minev, Mario Motta, Bibek Pokharel, Pedro Rivero, Kunal Sharma, Christopher J. Wood, Ali Javadi-Abh

The estimation of low energies of many-body systems is a cornerstone of computational quantum sciences. Variational quantum algorithms ca
states on pre-fault-tolerant quantum processors, but their lack of convergence guarantees and impractical number of cost function estimation
experiments to large systems. Alternatives to variational approaches are needed for large-scale experiments on pre-fault-tolerant devices. Her
quantum processor to compute eigenenergies of quantum many-body systems on two-dimensional lattices of up to 56 sites, using the Krylov
algorithm, an analog of the well-known classical diagonalization technique. We construct subspaces of the many-body Hilbert space using Trot


arXiv > quant-ph > arXiv:2405.05068

Quantum Physics

[Submitted on 8 May 2024]

**Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer**

Javier Robledo-Moreno, Mario Motta, Holger Haas, Ali Javadi-Abhari, Petar Jurcevic, William Kirby, Simon Martiel, Kunal Sh
Shirakawa, Iskandar Sitdikov, Rong-Yang Sun, Kevin J. Sung, Maika Takita, Minh C. Tran, Seiji Yunoki, Antonio Mezzacapo

A universal quantum computer can be used as a simulator capable of predicting properties of diverse quantum systems. Electronic structur
practical use cases around the hundred-qubit mark. This appears promising since current quantum processors have reached these sizes. H
onto quantum computers yields deep circuits, and for for pre-fault-tolerant quantum processors, the large number of measurements to es
prohibitive runtimes. As a result, realistic chemistry is out of reach of current quantum computers in isolation. A natural question is whethe
computation can relieve quantum processors from parsing all but a core, intrinsically quantum component of a chemistry workflow. Here, w

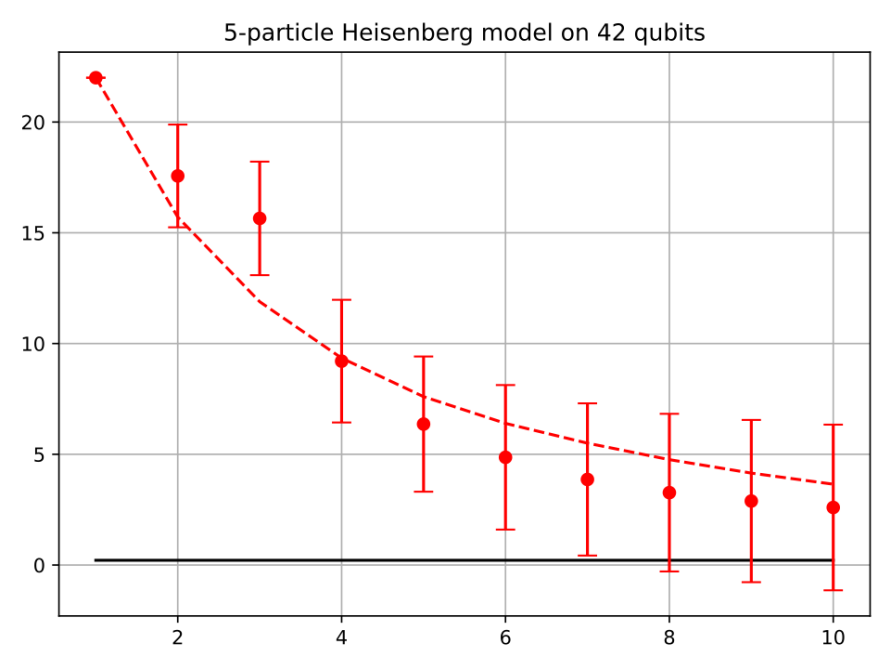
# Expt #1: diagonalization of large many-body systems on a quantum processor

**Goal:** estimate ground state energy of quantum Hamiltonian.

Classically challenging due to exponential Hilbert space dimension*.

**Outline of this section:**

1. Overview of Krylov Quantum Diagonalization (KQD)
2. Experimental results




*Assuming general, hard case: sufficiently entangled, supported on exponentially-many basis states, etc.

# Lanczos/Arnoldi method

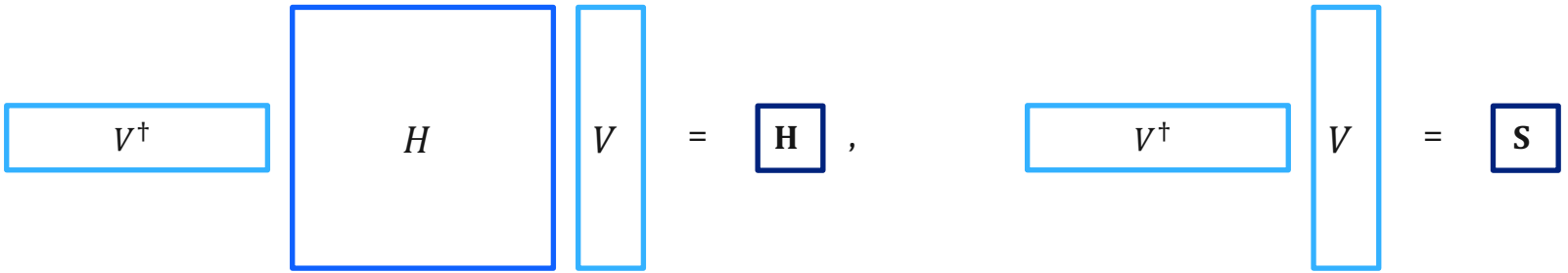
= classical method for approximating lowest eigenvalues.

**(Very) high-level idea:**

1. Initial guess $|\psi_0\rangle \Rightarrow H|\psi_0\rangle \Rightarrow \cdots \Rightarrow H^{D-1}|\psi_0\rangle$

2. $(\mathbf{H}, \mathbf{S})$ = project $H$ onto span$\underbrace{[|\psi_0\rangle, H|\psi_0\rangle, H^2|\psi_0\rangle, \ldots, H^{D-1}|\psi_0\rangle]}_{\mathrm{V}}$

Krylov space




3. Lowest eigenvalue of $(\mathbf{H}, \mathbf{S})$ i.e., of $\mathbf{Hv} = \lambda\mathbf{Sv}$, approximates lowest eigenvalue of $H$

# Lanczos/Arnoldi method

Caveat: typically in classical Lanczos(-like) methods, would orthogonalize along the way… challenging in quantum implementations.

**Advantage:** converges exponentially with D (in ∞ precision arithmetic).

**Disadvantage:** classically, requires storing entire statevectors $H^i|\psi_0\rangle$ ⇒ exponential overhead.

*Can we construct a quantum version that mitigates statevector overhead while keeping fast convergence?*[1]

Recent review!

[1] Parrish and McMahon, https://arxiv.org/abs/1909.08925; Motta *et* al., https://arxiv.org/abs/2312.00178; and many more!

# Quantum “Lanczos method” = “Quantum Krylov”

**Options for generating Krylov space:** multiply $|\psi_0\rangle$ by…

- Powers of $H$ — same as original Lanczos ⇒ nontrivial on quantum but possible in principle.[1]
- $e^{-Hkdt}$ — this version claimed “Qlanczos.”[2]
- $T_k(H)$ — arises naturally from block encoding.[3]
- $e^{iHkdt}$ — many good options e.g. Trotterization, qubitization, etc.

Will focus on last version in this talk.

[1]Seki and Yunoki, PRX Quantum 2, 010333 (2021); [2]Motta *et al.*, Nat. Phys. 16, 205–210 (2020); [3]Kirby *et al.*, Quantum 7, 1018 (2023).

# Krylov Quantum Diagonalization with real time-evolutions

Majority of works have focused on Krylov states generated by real time-evolution:

$$V = [|\psi_0\rangle, U|\psi_0\rangle, U^2|\psi_0\rangle, \ldots, U^{D-1}|\psi_0\rangle] \text{ for } U = e^{iHdt}$$

Need to estimate on quantum computer

$$\mathbf{H_{jk}} = \langle\psi_0|(U^j)^\dagger H U^k|\psi_0\rangle,$$

$$\mathbf{S_{jk}} = \langle\psi_0|(U^j)^\dagger U^k|\psi_0\rangle$$

for each $j, k = 0,1,\ldots,D-1$,

then classically calculate lowest eigenvalue of $\mathbf{Hv} = \lambda\mathbf{Sv}$ ⇒output.

# Aside: generalized eigenvalue problems

Regular eigenvalue problem: $\mathbf{H}v = \lambda v$

Generalized eigenvalue problem: $\mathbf{H}v = \lambda \mathbf{S}v$

"Eigenvalue problem in non-orthonormal basis" ⇒ inner product is $v^\dagger \boldsymbol{S} v$, not $v^\dagger v$

Usually solve by converting to regular eigenvalue problem, e.g., $\boldsymbol{S}^{-1}\boldsymbol{H}v = \lambda v$

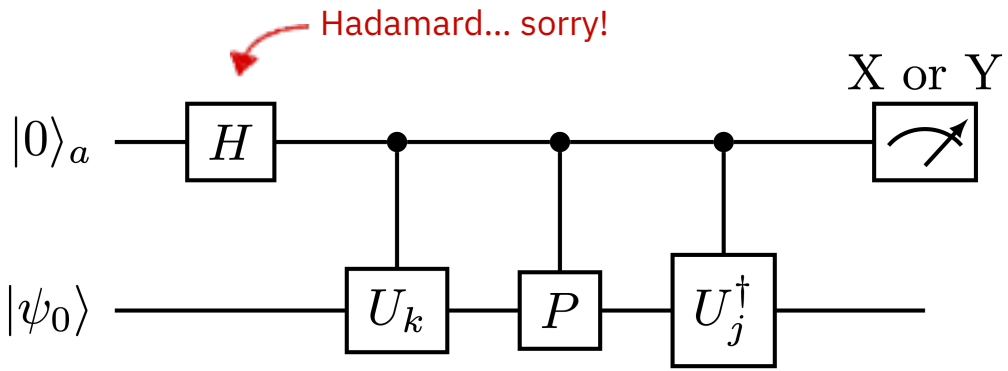
...but

here be dragons: if $\boldsymbol{S}$ is ill-conditioned, then inverting it requires caution

# Estimating matrix elements (basic version)

Targets: $\mathbf{H_{jk}} = \langle\psi_0|(U^j)^\dagger H U^k|\psi_0\rangle, \quad \mathbf{S_{jk}} = \langle\psi_0|(U^j)^\dagger U^k|\psi_0\rangle\,.$

Can approach using Hadamard test:

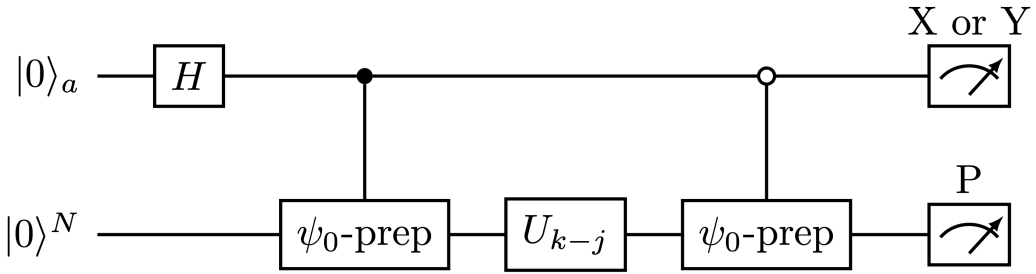



Yields $\langle X\rangle_a = Re[\langle\psi_0|(U^j)^\dagger P U^k|\psi_0\rangle], \quad \langle Y\rangle_a = Im[\langle\psi_0|(U^j)^\dagger P U^k|\psi_0\rangle]$

# Estimating matrix elements (better version)

Change target: $\mathbf{H_{jk}} = \langle\psi_0|HU^{k-j}|\psi_0\rangle$, $\mathbf{S_{jk}} = \langle\psi_0|U^{k-j}|\psi_0\rangle$ for $k \geq j$ (below diag. use Hermitianity)

- Note: equal to ideal matrix elements if time-evolution exact.




This assumes $U^{k-j}$ preserves particle number; given this, expectation values come out to

$$\langle X \otimes P\rangle = Re\left[e^{-i\phi}\langle\psi_0|PU|\psi_0\rangle\right], \langle Y \otimes P\rangle = Im\left[e^{-i\phi}\langle\psi_0|PU|\psi_0\rangle\right].$$

classically-calculable phase from $U^{k-j}|0\rangle^N = e^{i\phi}|0\rangle^N$

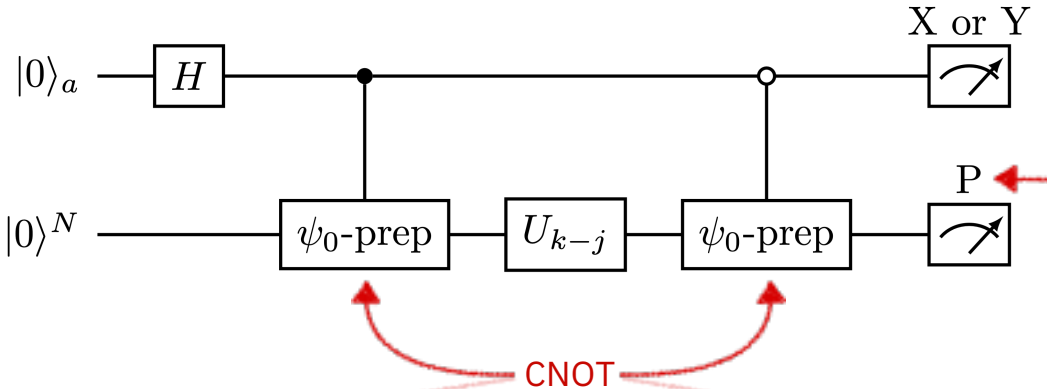
This circuit is the starting point for our experiment.

# Theory of KQD with real time-evolutions

**Summary:**

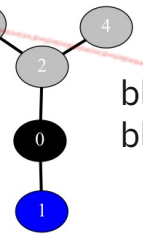
- Estimate $\mathbf{H_{jk}}$, $\mathbf{S_{jk}}$ via Hadamard(-ish) tests and repeated sampling.
- Depending on Hamiltonian, can avoid controlled time-evolutions using symmetry (particle number).
- Advantage: can use crude approximations for time-evolution to get **low circuit depth**.
- Time-evolution always approximated — more accuracy requires more depth.

# Experiments: single particle example

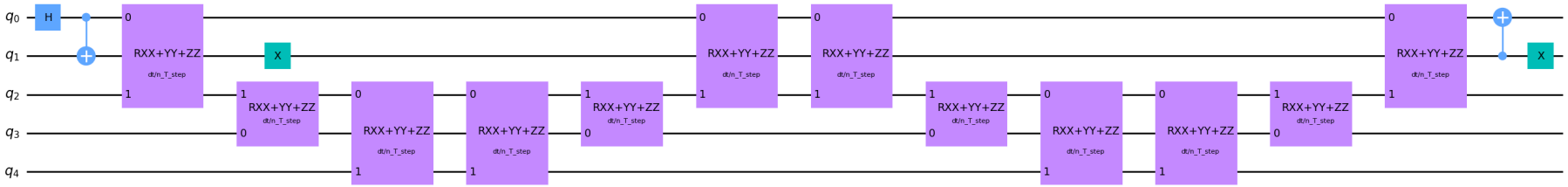



$$H = \sum_{\langle i,j \rangle} \left( X_i X_j + Y_i Y_j + j_2 Z_i Z_j \right)$$

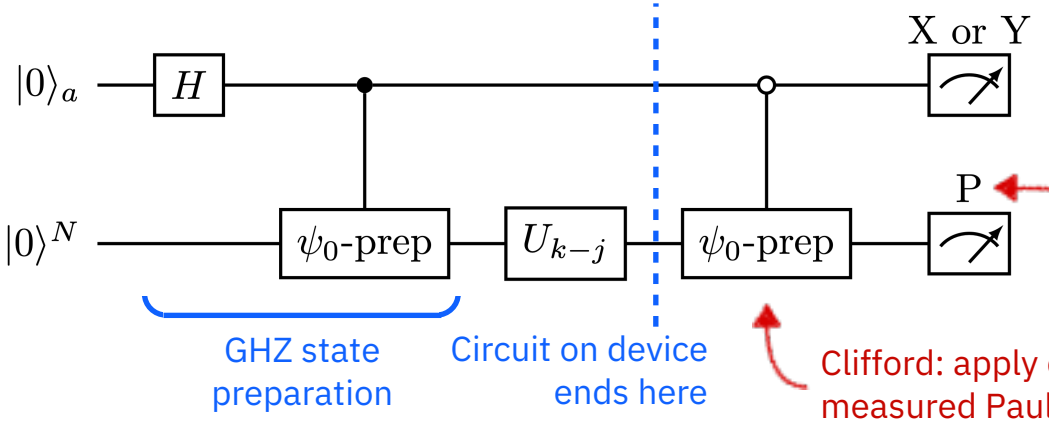
- 1-particle example: $|\psi_0\rangle = |100\ldots0\rangle$
- $U^{k-j}$ approximated by 2 2nd-order Trotter steps
- Example circuit (only on 4 system qubits):




blue = control,
black = initial excitation



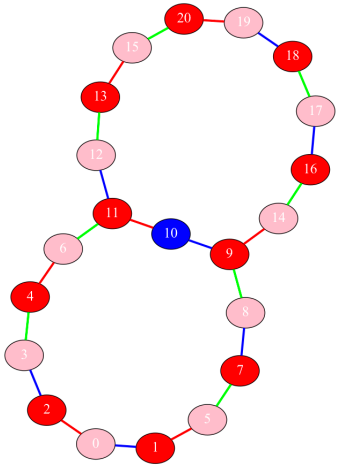
# Experiments: k-particle subspaces




$$H = \sum_{\langle i,j \rangle} \left( X_i X_j + Y_i Y_j + j_2 Z_i Z_j \right)$$

Clifford: apply classically to measured Pauli observables, yielding $2(k+2)$ measurement bases

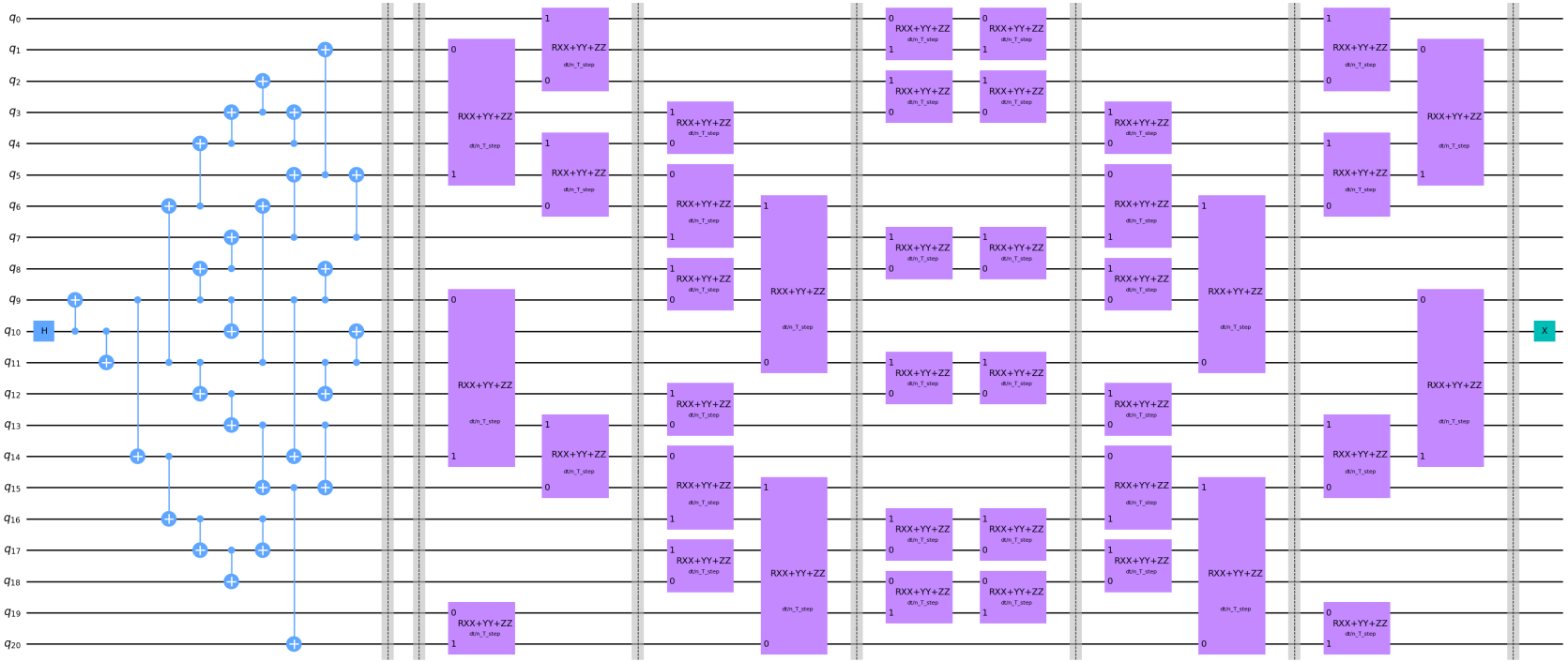
- 10-particle example: $|\psi_0\rangle = |101010\ldots10\rangle$
- $U^{k-j}$ approximated by $r$ Trotter steps
  - 20 qubit example:




blue = control,
red = initial excitation,
edge colors = 2Q layers

- Corresponding circuit looks like...

# 10-particle example




*extra complication: creating few unique layers

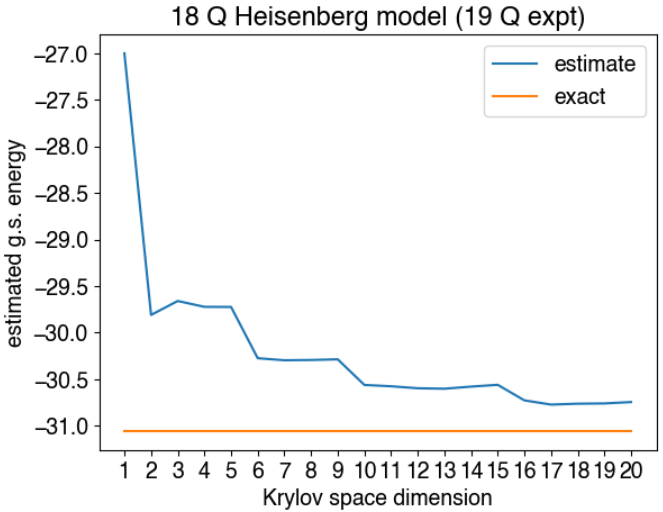
# Aside: error analysis in the presence of noise

Can show[1] that energy error from a noisy quantum Krylov experiment is bounded as

$$\text{energy error} \leq O\left(\delta' + \frac{\|H\|}{|\gamma_0|^2}\left[\left(\frac{1}{\delta'-\delta}\right)\eta + \left(1-\frac{\pi\delta}{2\|H\|}\right)^{-D}\right]\right)$$

from free parameter | from noise | from Krylov projection $\propto (1+\beta)^{-D}$

So one expects a result with this overall shape:




- $\gamma_0$ = noise rate
- $\eta$ = initial state overlap
- $D$ = spectral gap
- $\Delta$ = Krylov dimension
- $\delta$ , $\delta'$ = positive free parameters

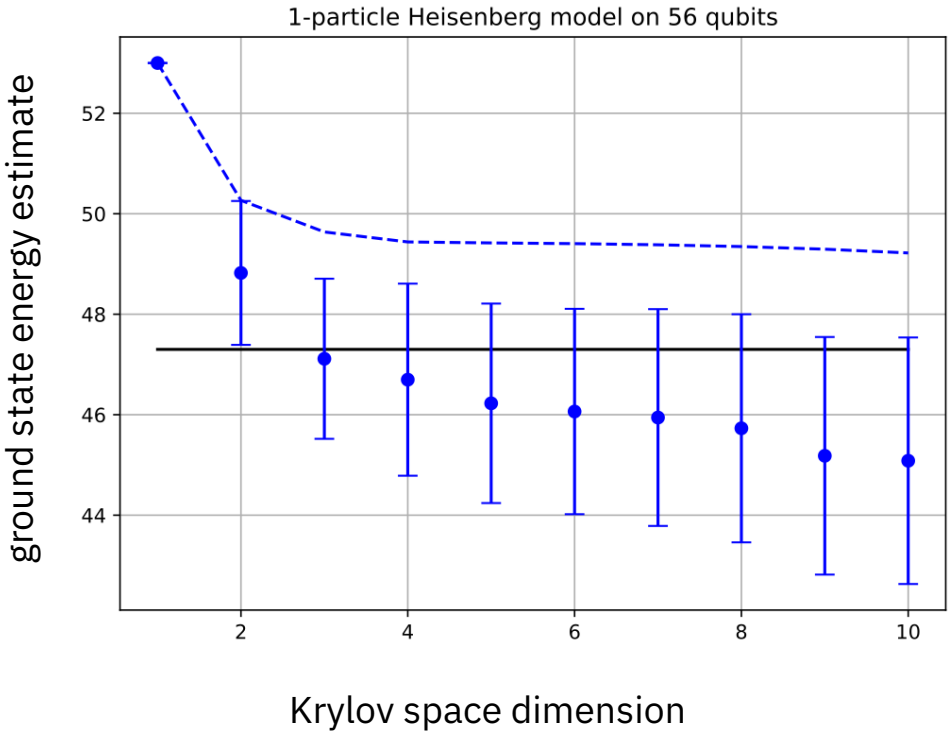
**Plot**

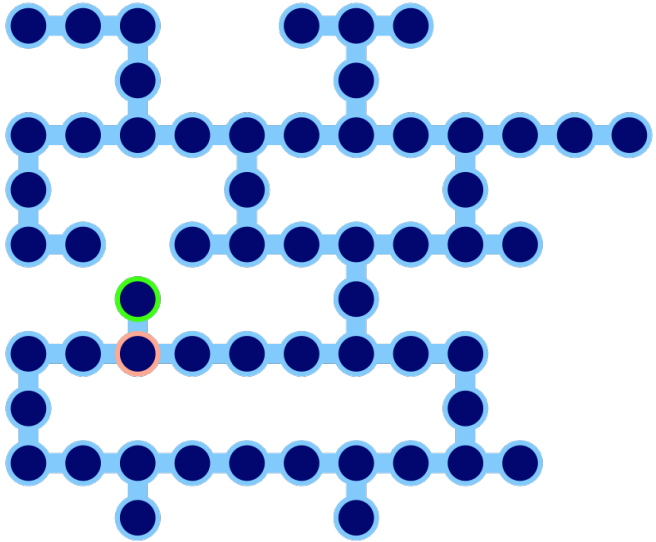
- Classical simulation, 2D Heisenberg model on heavy hex + sparse nonlocal interactions (1 swap)
- $4D = 80$ circuits in total
- $10^6$ shots per circuit
- CNOT-depth$= 26$

[1]Epperly *et al.*, https://arxiv.org/abs/2110.07492, Kirby, https://arxiv.org/abs/2401.01246

# 1-particle experimental results (56+1 qubits)

**Target Hamiltonian:** $H = \sum_{\langle i,j \rangle} \left( X_i X_j + Y_i Y_j + j_2 Z_i Z_j \right)$ with $\langle i,j \rangle$ ~nearest neighbor on heavy-hex subgraph

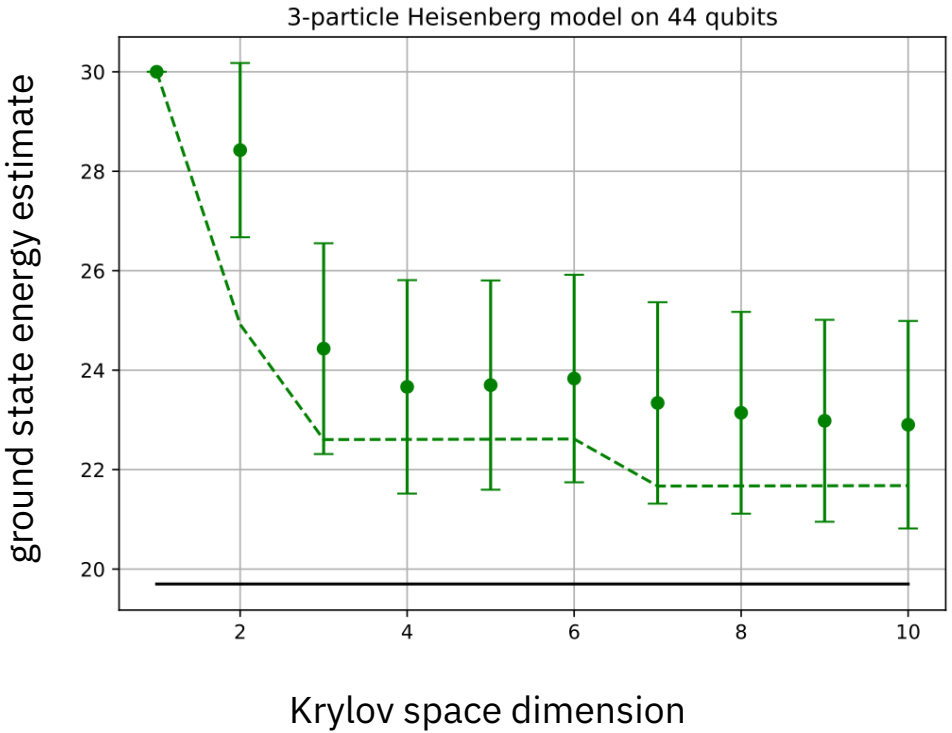


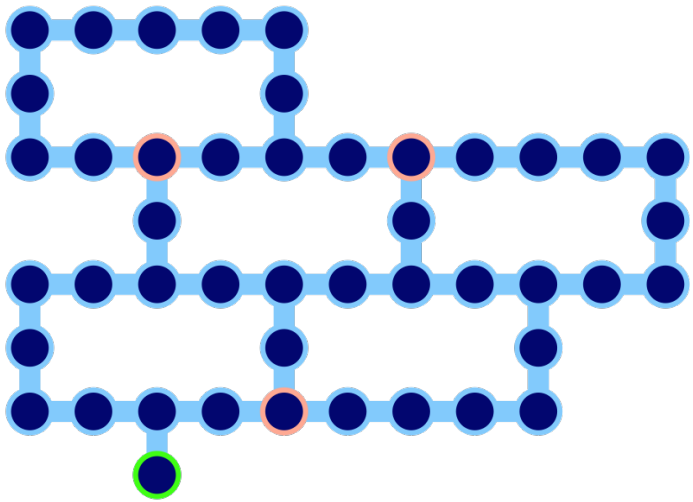



Green = control qubit
Red = initial excitation

# 3-particle experimental results (44+1 qubits)

**Target Hamiltonian:** $H = \sum_{\langle i,j \rangle} \left( X_i X_j + Y_i Y_j + j_2 Z_i Z_j \right)$ with $\langle i,j \rangle$ ~nearest neighbor on heavy-hex subgraph

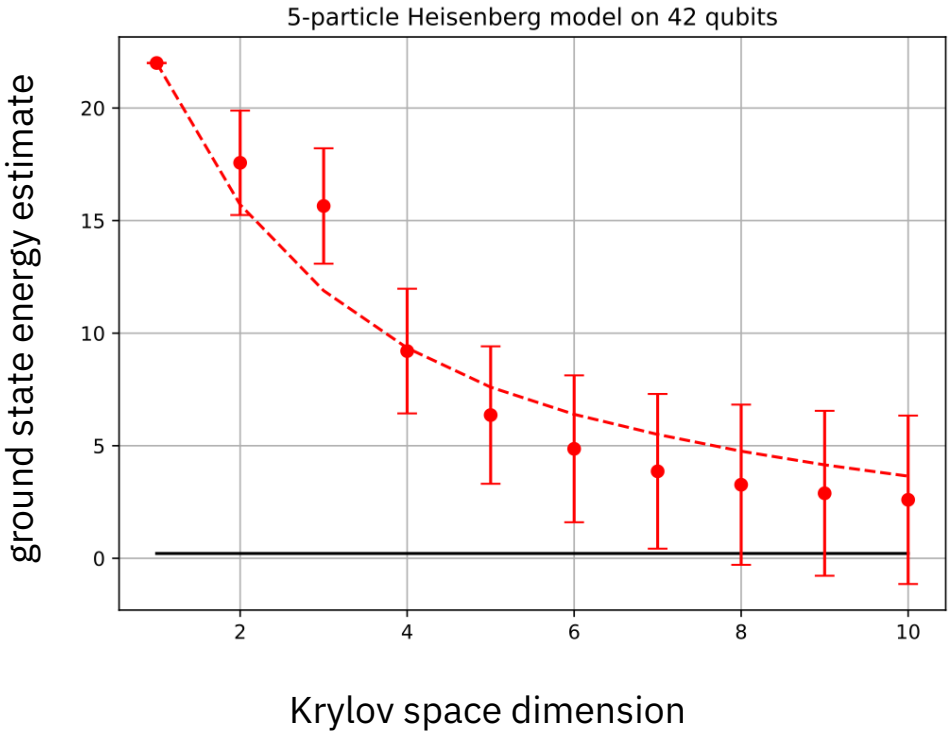


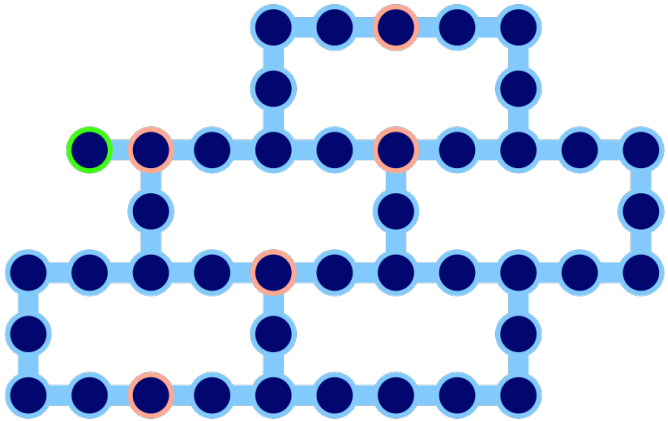



Green = control qubit
Red = initial excitation

# 5-particle experimental results (42+1 qubits)

**Target Hamiltonian:** $H = \sum_{\langle i,j \rangle} \left( X_i X_j + Y_i Y_j + j_2 Z_i Z_j \right)$ with $\langle i,j \rangle$ ~nearest neighbor on heavy-hex subgraph



Green = control qubit
Red = initial excitation