Institut de Ciències del Cosmos
UNIVERSITAT DE BARCELONA

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Quantum Krylov Algorithm

Applied to the NSM

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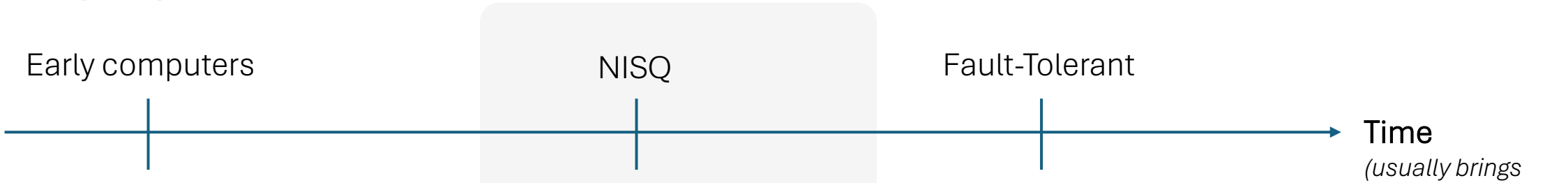
Barcelona, January 26th

Introduction

How can *quantum computers* be useful?

Timeline



VQE
- Parametrized circuit
- Minimized by brute force
- Access directly wavefunction (gs)

Time evolution

Subspace expansion Methods

…

QPE
- Energy spectra

Shor's algorithm
- Break RSA

…

Subspace expansion Methods

low/high energy sub-space expansion of the *Hamiltonian*

Idea

- Propose ***wavefunctions***
- Use ***Quantum Computers*** to change basis

→ Same as ***classical*** Krylov !

Introduction

classical Krylov

Given *H* and a reference state, define subspace

$$\mathcal{K} = \text{span}\{|\psi\rangle, H|\psi\rangle, H^2|\psi\rangle, ...\}$$

Expand *H* in this subspace

$$\tilde{H} = VHV^\dagger$$

where *V* is formed by orthogonal vector in the subspace, and solve for *H*

$$\hat{H}^n = \sum_i \lambda_i^n |\psi_i\rangle$$

Introduction

classical Krylov

$$\mathcal{K} = \text{span}\{|\psi\rangle, H|\psi\rangle, H^2|\psi\rangle, ...\}$$

$$\tilde{H} = VHV^\dagger$$

Key Ingredients:

- Generating a basis close to ***subspace***
- Change of basis for the ***operator*** of interest

Quantum Krylov

Key Ingredients

- *Generating* a basis

Hamiltonians are *not* unitary!

- *Change* of basis

Non orthogonal basis!

- *Time-evolved* states $f(H) = \exp(iH\mathrm{d}t)$

$$\mathcal{K} = \{|\psi\rangle, e^{iH\mathrm{d}t}|\psi\rangle, e^{2iH\mathrm{d}t}|\psi\rangle, ...\}$$

- *Expectation values* with

$$\tilde{H}_{ij} = \langle\psi_i|H|\psi_j\rangle$$

How do we solve this?

Propose a generalized eigenvalue problem:

$$\hat{H}v = \lambda\hat{S}v$$

where

$$S_{ij} = \langle\psi_i|\psi_j\rangle$$

Circuit proposal

Key Ingredients

- *Time-evolved* states $f(H) = \exp(iH\mathrm{d}t)$

$$\mathcal{K} = \{|\psi\rangle, e^{iH\mathrm{d}t}|\psi\rangle, e^{2iH\mathrm{d}t}|\psi\rangle, \ldots\}$$

- *Expectation values* with

$$\tilde{H}_{ij} = \langle\psi_i|H|\psi_j\rangle$$
$$S_{ij} = \langle\psi_i|\psi_j\rangle$$

Article

https://doi.org/10.1038/s41467-025-59716-z

Krylov diagonalization of large many-body Hamiltonians on a quantum processor

Received: 26 January 2025

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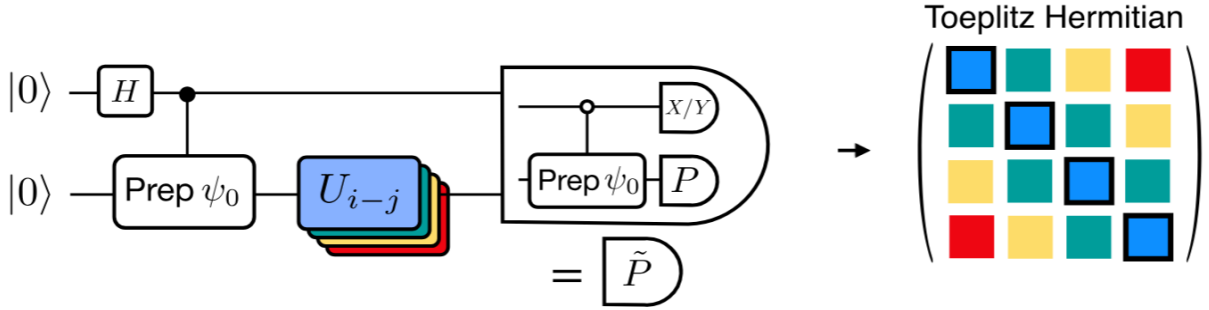
Published online: 24 June 2025

Check for updates

Nobuyuki Yoshioka[1,2,10], Mirko Amico[3,10], William Kirby[3,10], Petar Jurcevic[3], Arkopal Dutt[4], Bryce Fuller[3], Shelly Garion[5], Holger Haas[3], Ikko Hamamura[6,7], Alexander Ivrii[5], Ritajit Majumdar[8], Zlatko Minev[3], Mario Motta[3], Bibek Pokharel[9], Pedro Rivero[3], Kunal Sharma[3], Christopher J. Wood[3], Ali Javadi-Abhari[3] & Antonio Mezzacapo[3]



Yoshioka, N., Amico, M., Kirby, W. *et al. Nat Commun* **16**, 5014 (2025).

Circuit proposal

Key Ingredients

- *Time-evolved* states $f(H) = \exp(iH\mathrm{d}t)$

$$\mathcal{K} = \{|\psi\rangle, e^{iH\mathrm{d}t}|\psi\rangle, e^{2iH\mathrm{d}t}|\psi\rangle, \ldots\}$$

- *Expectation values* with

$$\tilde{H}_{ij} = \langle\psi_i|H|\psi_j\rangle$$
$$S_{ij} = \langle\psi_i|\psi_j\rangle$$

Exact time evolution is expensive!
(*Use Trotter decomposition*)

Results

Results

Exact exponential ^{20}Ne

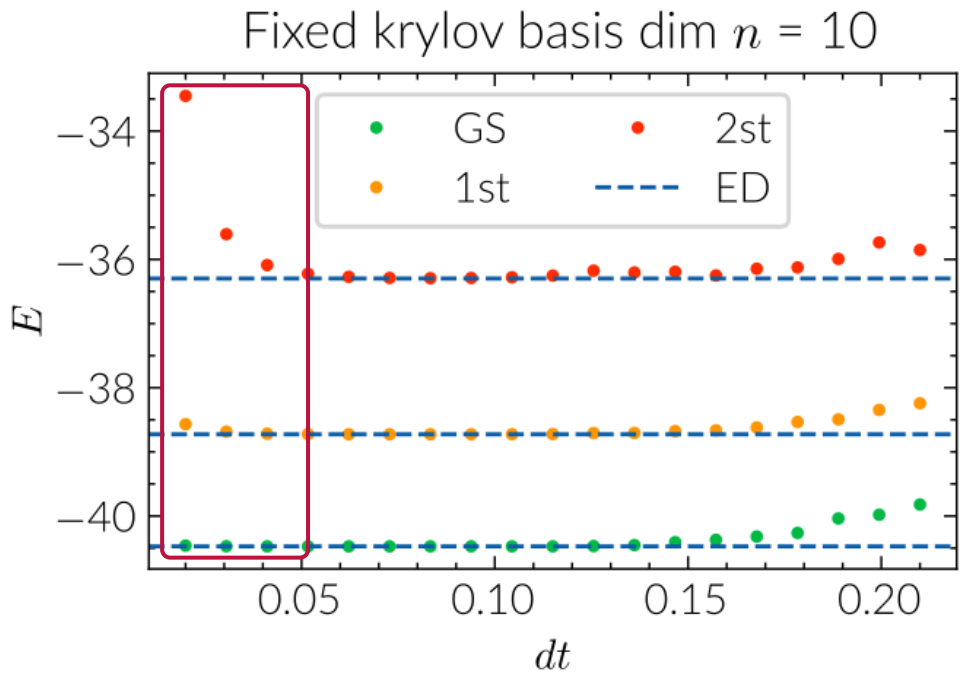
Check efficiency of the basis

Trotterized exponential ^{8}Be

Check effect of Trotter error affects

NSM results

Exact exponential ^{20}Ne



Results

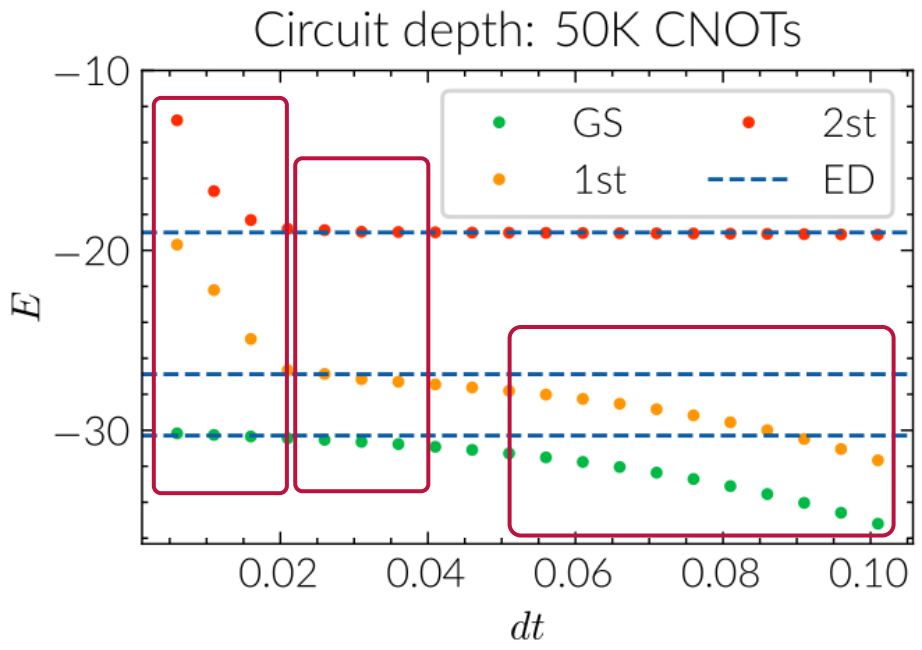
- Explore Hilbert space
- Aliasing effects (due to complex exponential)

Trotterized exponential ^{8}Be

NSM results

Exact exponential ^{20}Ne

Trotterized exponential ^{8}Be



Results

- Limited from ***below***: explore Hilbert space
- Limited from ***above***: Trotter error

Fine tuning of Krylov dimension

NSM results

Exact exponential ^{20}Ne

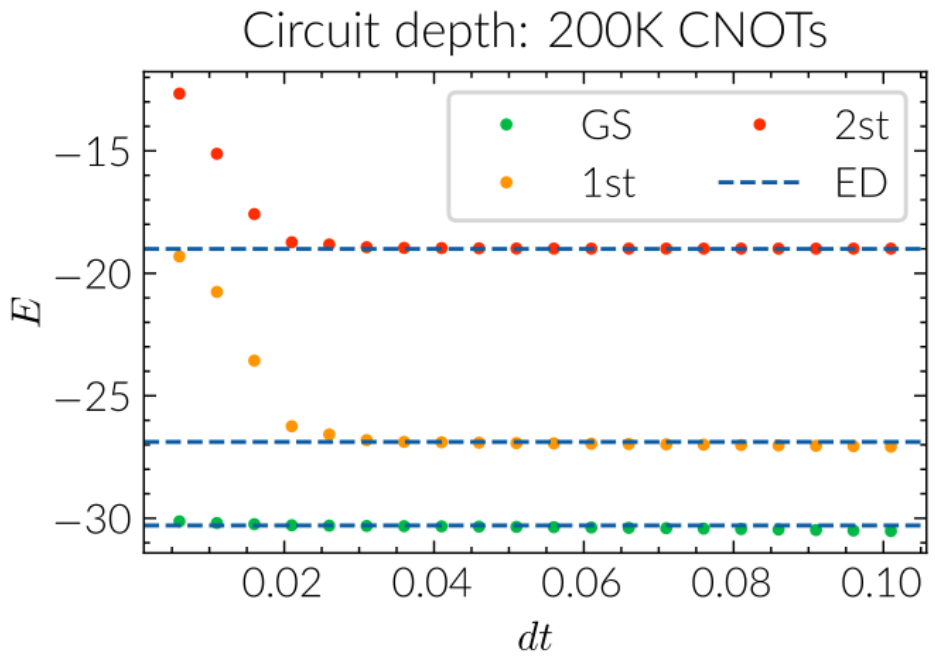
Trotterized exponential ^{8}Be

More gates

↓

Reduce Trotter error

Need in 10^5 CNOT gates *(not feasible)*



Conclusions

Conclusions

Not available *yet*

Easy solution

Wait for *better* computers

Difficult solution

- Improve time evolution
  - Q. Phase Estimation
  - Rodeo algorithm
  - Krylov
  - Adiabatic
- Find *other* subspace to expand H

Backup

Introduction

classical Krylov

$$\mathcal{K} = \text{span}\{|\psi\rangle, H|\psi\rangle, H^2|\psi\rangle, ...\}$$

$$\tilde{H} = VHV^\dagger$$

This works because:

- Rayleigh principle
- Gram-Schmidt
  - Create orthogonal basis
- Optimized version: create tridiagonal matrix for transformation, highly efficient to solve…
  - Only save some vectors

Key ingredients:

- Generating a basis with ***operator*** (encode of eigenvectors)
- Change basis of the ***operator*** of interest (encode the eigenvalues)

Or functions of the operator!

Also forget about requirements for classical optimization

- Classical:

Advantages

- Directly implement powers of H
- Create an **orthonormal** basis
- More flexibility on operation

Disadvantages

- Memory: save vectors and matrix (sparse?)
- Slow calculations: grow with dimensionality

- Quantum:

Advantages

- Inherently tackle **large** dimension
- Some functions of the operator are **efficient** to implement

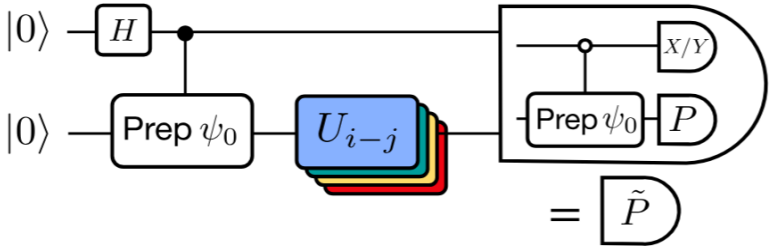
Disadvantages

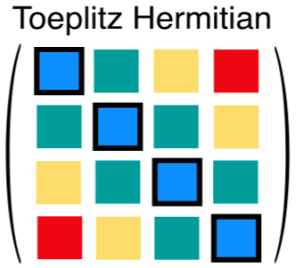
- Hamiltonians are not (usually) unitary
- Creating an orthonormal basis is not easy

Circuit proposal

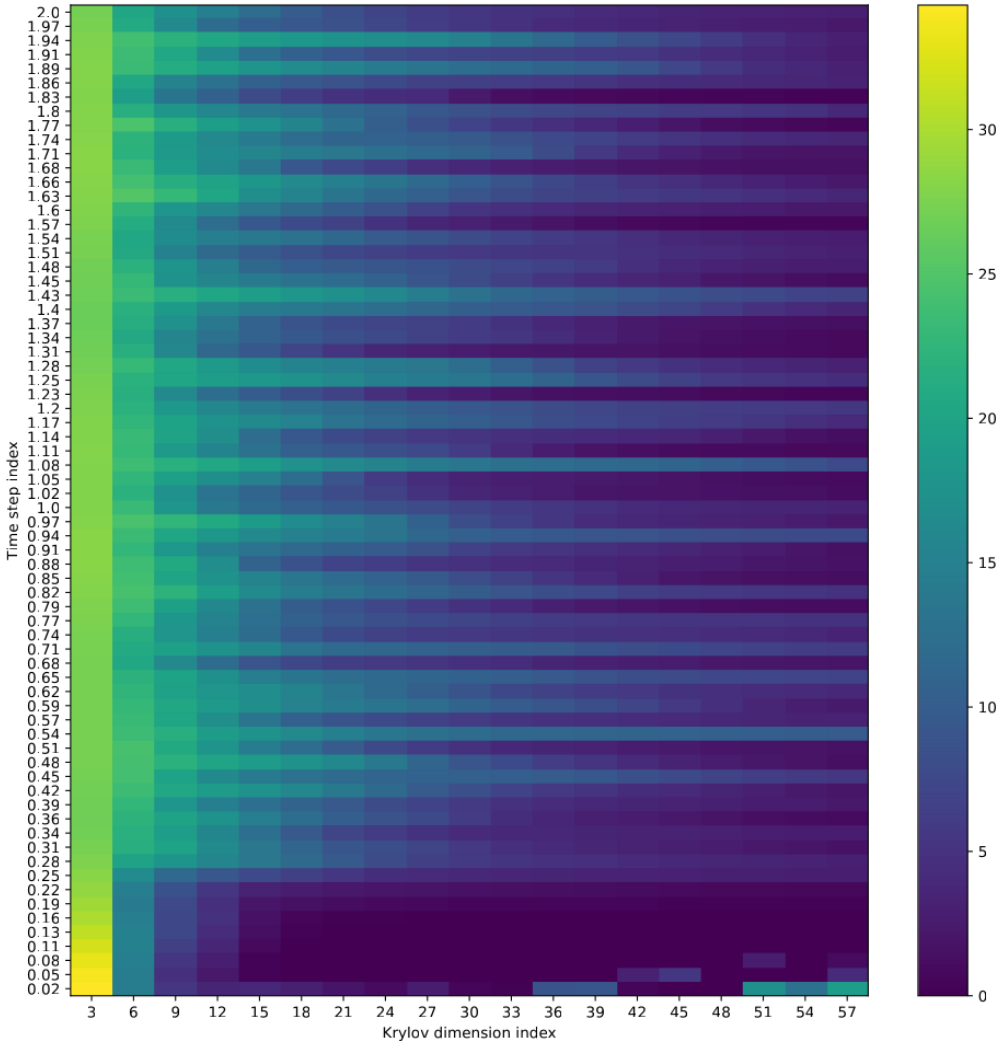
$$
\begin{aligned}
|0\rangle_a|0\rangle^N &\xrightarrow{\hat{H}} \frac{1}{\sqrt{2}}\left(|0\rangle_a|0\rangle^N + |1\rangle_a|0\rangle^N\right) \\
&\xrightarrow{\text{1-ctrl-prep}} \frac{1}{\sqrt{2}}\left(|0\rangle_a|0\rangle^N + |1\rangle_a|\psi_0\rangle\right) \\
&\xrightarrow{U_{k-j}} \frac{1}{\sqrt{2}}\left(e^{i\phi}|0\rangle_a|0\rangle^N + |1\rangle_a U_{k-j}|\psi_0\rangle\right) \\
&\xrightarrow{\text{0-ctrl-prep}} \frac{1}{\sqrt{2}}\left(e^{i\phi}|0\rangle_a|\psi_0\rangle + |1\rangle_a U_{k-j}|\psi_0\rangle\right)
\end{aligned}
$$

$$
\begin{aligned}
\tilde{H}_{ij} = \langle\psi_i|H|\psi_j\rangle &= \langle\psi_0|\exp iH(it)H\exp iH(jt)|\psi_0\rangle \\
&= \langle\psi_0|H\exp iH(j-i)t|\psi_0\rangle
\end{aligned}
$$

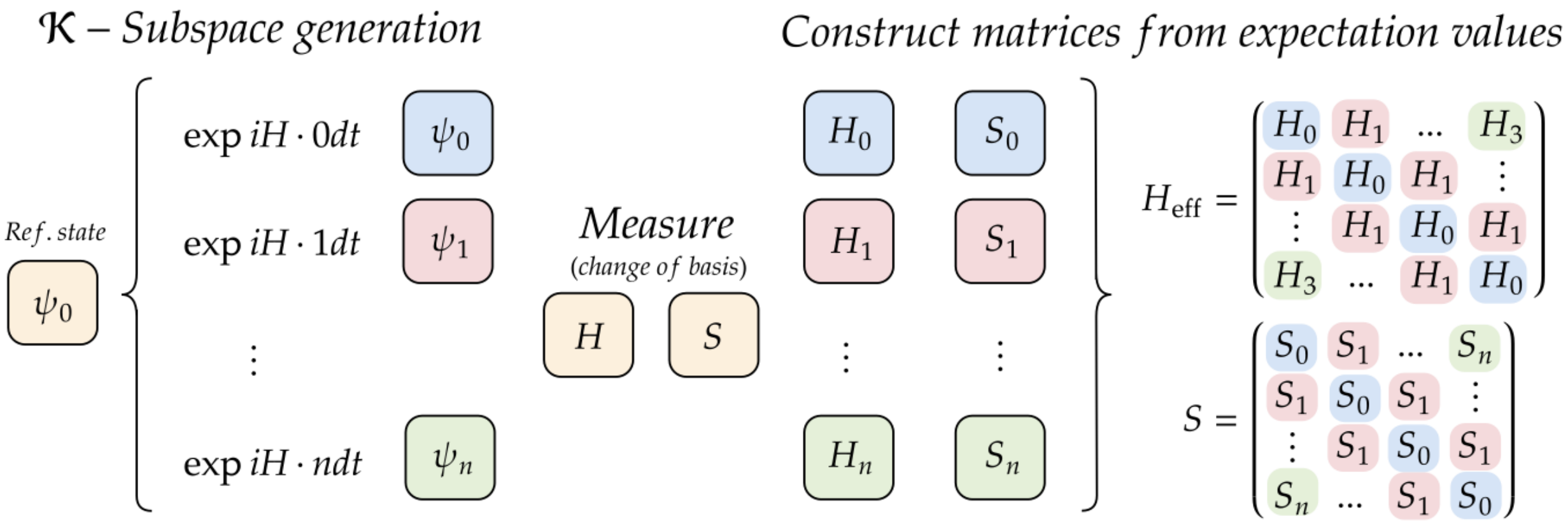




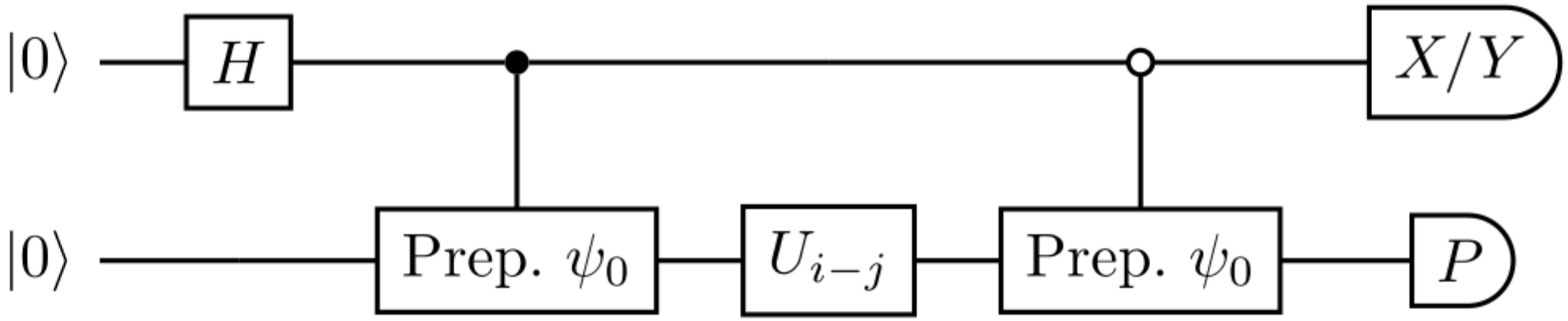
Kyrlov dimension



Algorithm overview



Circuit



All – to-all connectivity

Efficient quantum circuits for quantum computational chemistry

Yordan S. Yordanov,[1] David R. M. Arvidsson-Shukur,[1,2] and Crispin H. W. Barnes[1]
[1]*Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge CB3 0HE, United Kingdom*
[2]*Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

(Received 21 August 2020; accepted 17 November 2020; published 21 December 2020)

Molecular quantum simulations with the variational quantum eigensolver (VQE) rely on ansatz states that approximate the molecular ground states. These ansatz states are generally defined by parametrized fermionic excitation operators and an initial reference state. Efficient ways to perform fermionic excitations are vital for the realization of the VQE on noisy intermediate-scale quantum computers. Here, we address this issue by first demonstrating circuits that perform qubit excitations, excitations that do not account for fermionic anticommutation relations. We then extend the functionality of these circuits to perform fermionic excitations. Compared to circuits constructed with the standard use of "*CNOT* staircases", our circuits offer a linear reduction in the number of *CNOT* gates, by a factor of 2 (8) per single (double) qubit or fermionic excitation, respectively. Our results reduce the requirements for near-term realizations of quantum molecular simulations.

DOI: 10.1103/PhysRevA.102.062612

Trotterized exponential

- ^{8}Be: 10 time-steps, dt = 0.01

```
[-30.33953926 -26.91793339 -18.99281409 -15.84926013 -11.88931861]
[-30.29539461 -26.88369692 -19.0041005  -15.86699708 -15.31298892]
```

2nd order Trotter step:

20K CNOT 5 K (rely on full connectivity)

NSM results

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```

2nd order Trotter step:

20K CNOT ⟶ 5 K (rely on full connectivity)

NSM

Remarks:

- Trotter error is huge

- ^{8}Be: 10 measurements, dt = 0.01, n = 10

```
[-30.33953926 -26.91793339 -18.99281409 -15.84926013 -11.88931861]
[-30.29539461 -26.88369692 -19.0041005  -15.86699708 -15.31298892]
```

- ^{8}Be: 10 measurements, dt = 0.05, n = 2

```
[-31.45817535 -27.77340342 -19.15038359 -15.99342614 -12.05785508]
[-30.29539461 -26.88369692 -19.0041005  -15.86699708 -15.31298892]
```

- ^{8}Be: 10 measurements, dt = 0.01 , n = 10, 1st order Trotter

```
[-29.08722997 -27.8406708  -17.12914133 -13.66366612  -9.48217617]
[-30.29539461 -26.88369692 -19.0041005  -15.86699708 -15.31298892]
```

Exact and efficient Lanczos method on a quantum computer

William Kirby[1,2], Mario Motta[3], and Antonio Mezzacapo[4]