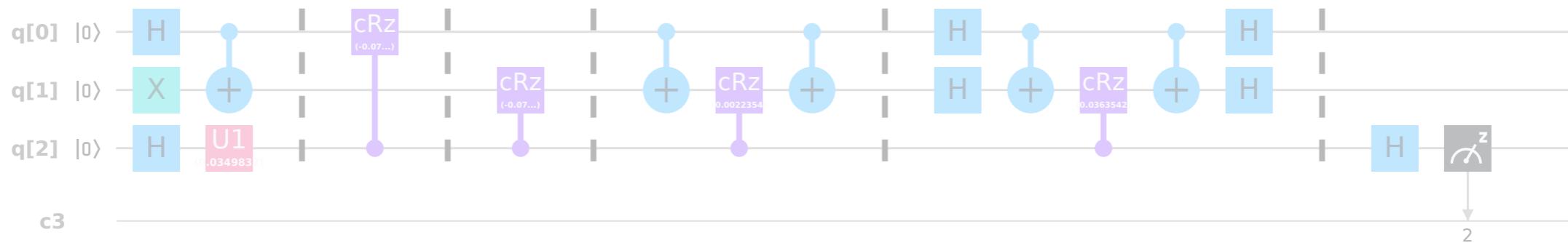


# Multireference Selected Quantum Krylov (MRSQK) Algorithm

# Renke Huang

## Feb 14, 2020



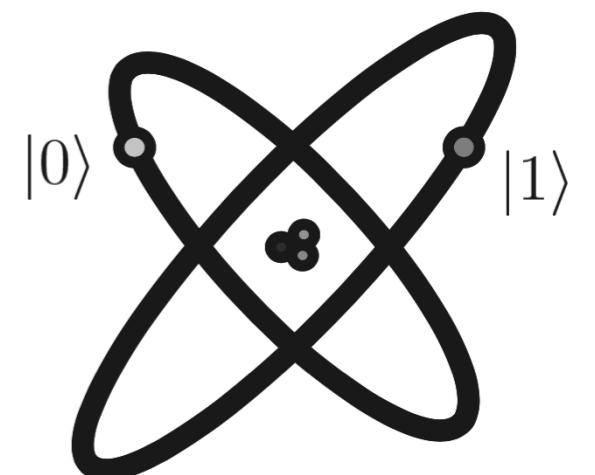
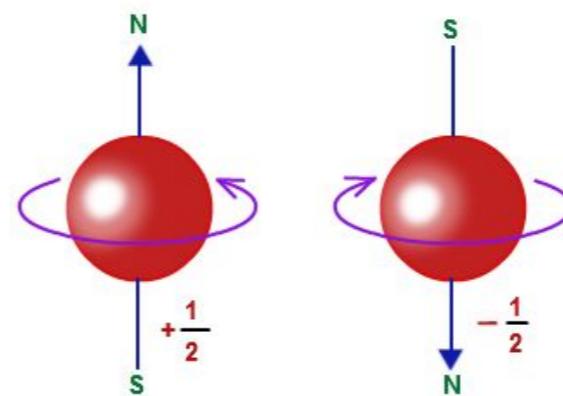
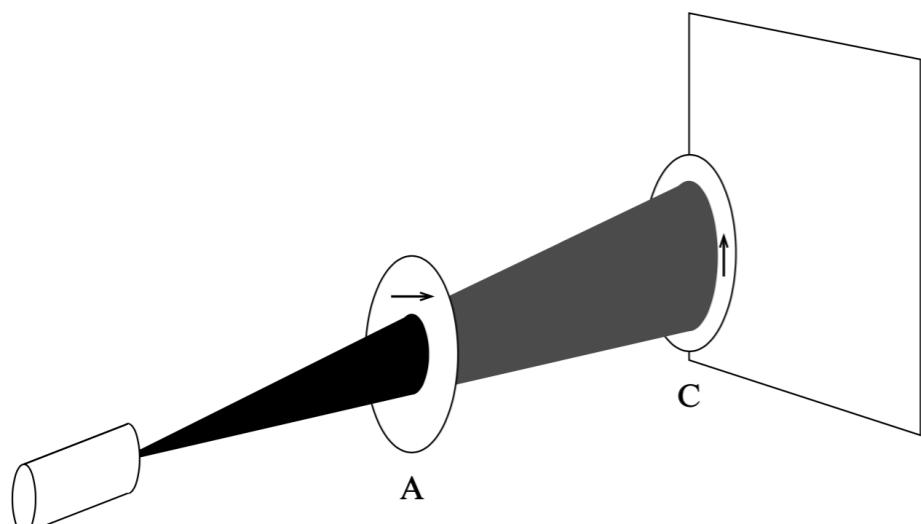
# What is a Quantum Computer?

**Qubit** unit state vector in a 2-dimensional complex vector (Hilbert) space  $V$

$$|u\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

**two-state quantum systems:**

photon polarization, electron spin, two electronic states of an atom



# What is a Quantum Computer?

**a Qubit** unit state vector in a 2-dimensional complex vector (Hilbert) space  $V$

$$|u\rangle = \alpha|0\rangle + \beta|1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

**n-Qubit** a unit state vector in the tensor product space of single qubit Hilbert spaces:  $V_{n-1} \otimes \dots \otimes V_1 \otimes V_0$

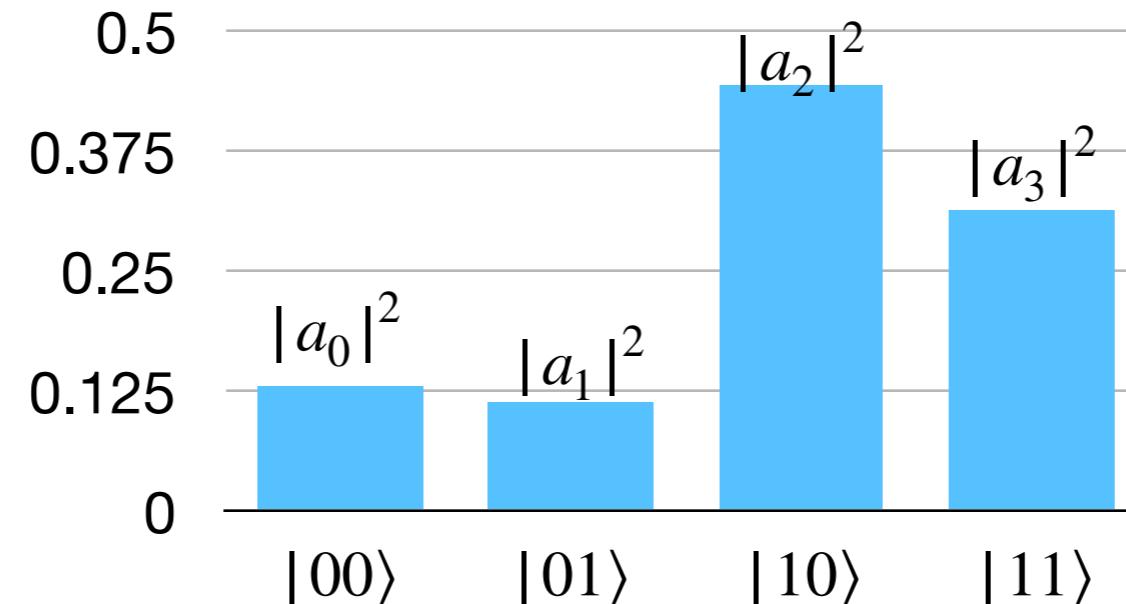
$$|\psi\rangle = a_0|0\dots00\rangle + a_1|0\dots01\rangle + \dots + a_{2^n-1}|1\dots11\rangle$$

$2^n$  computational basis states

store FCI vector!

**Measurement**

Probabilities

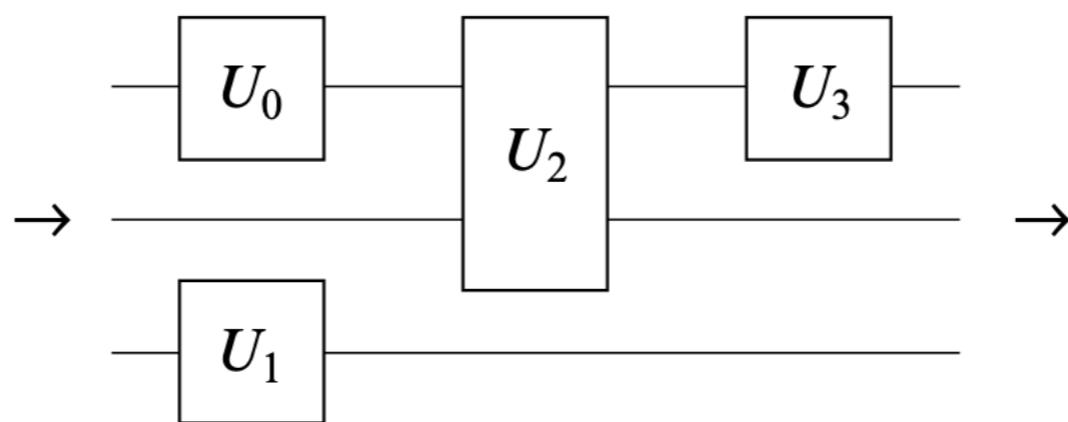


# How we do computations?

Quantum computer - a **closed** quantum system

**Quantum Algorithms** - **unitary transformations** of quantum systems

**quantum gates, quantum circuits**

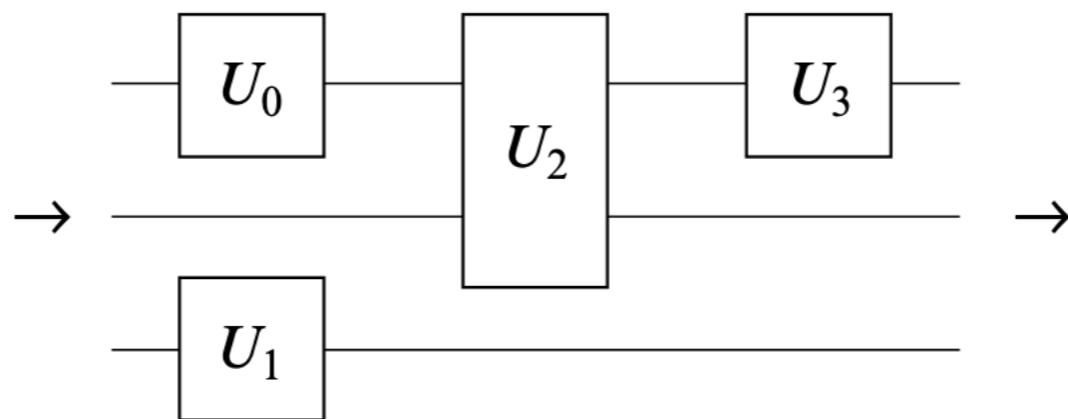


# How we do computations?

Quantum computer - a **closed** quantum system

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**Single qubit gates** (matrix representation in the computational basis)

$$\sigma^X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma^Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma^Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

**Multiple qubit gates**

$$\text{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

**Pauli gates/operators**

# Mapping fermions to qubits

Fermions (electrons)  
second quantization

$$a_p^\dagger |0\rangle = |1\rangle$$

$$a_p |1\rangle = |0\rangle$$

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$$\{a_p, a_q^\dagger\} = \delta_{pq}$$
$$\{a_p, a_q\} = \{a_p^\dagger, a_q^\dagger\} = 0$$



Qubits

$$\frac{\sigma_p^X - i\sigma_p^Y}{2} \otimes \sigma_{p-1}^Z \otimes \dots \otimes \sigma_0^Z$$

$$\frac{\sigma_p^X + i\sigma_p^Y}{2} \otimes \sigma_{p-1}^Z \otimes \dots \otimes \sigma_0^Z$$

# Mapping fermions to qubits

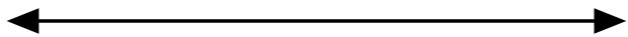
Fermions (electrons)  
second quantization

$$a_p^\dagger |0\rangle = |1\rangle$$

$$a_p |1\rangle = |0\rangle$$

$$\hat{H} = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

$$\begin{aligned}\{a_p, a_q^\dagger\} &= \delta_{pq} \\ \{a_p, a_q\} &= \{a_p^\dagger, a_q^\dagger\} = 0\end{aligned}$$



Qubits

$$\frac{\sigma_p^X - i\sigma_p^Y}{2} \otimes \sigma_{p-1}^Z \otimes \dots \otimes \sigma_0^Z$$

$$\frac{\sigma_p^X + i\sigma_p^Y}{2} \otimes \sigma_{p-1}^Z \otimes \dots \otimes \sigma_0^Z$$

$$\hat{H} = \sum_l^N h_l \bigotimes_{k=1}^{n_l} \sigma_{l_k}^{\{X,Y,Z\}}$$

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$$\Psi_f = a |0001\rangle + b |0010\rangle \\ + c |0100\rangle + d |1000\rangle$$

$$\{a_p, a_q^\dagger\} = \delta_{pq}$$

$$\{a_p, a_q\} = \{a_p^\dagger, a_q^\dagger\} = 0$$



Qubits

$$\frac{\sigma_p^X - i\sigma_p^Y}{2} \otimes \sigma_{p-1}^Z \otimes \dots \otimes \sigma_0^Z$$

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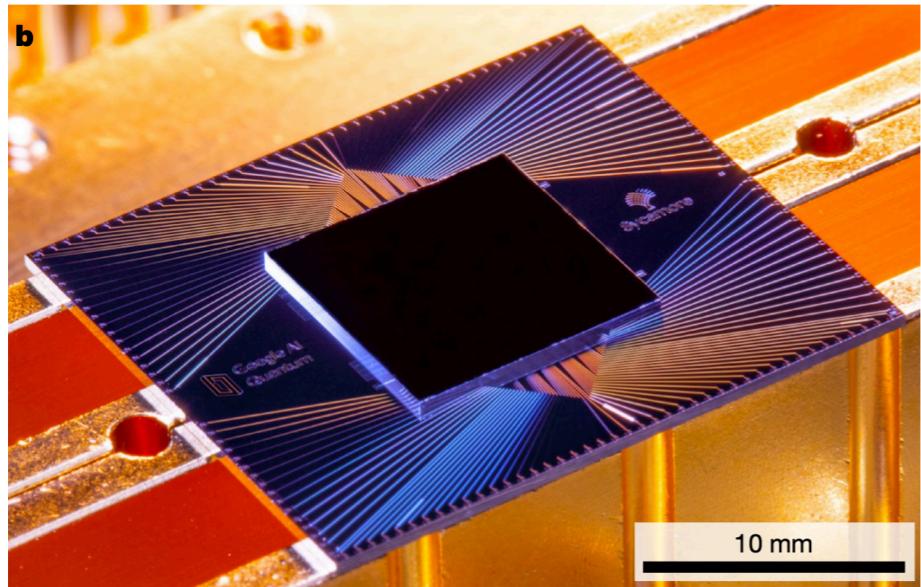
$$\hat{H} = \sum_l^N h_l \bigotimes_{k=1}^{n_l} \sigma_{l_k}^{\{X,Y,Z\}}$$

$$\Psi_q = a |0001\rangle + b |0010\rangle \\ + c |0100\rangle + d |1000\rangle$$

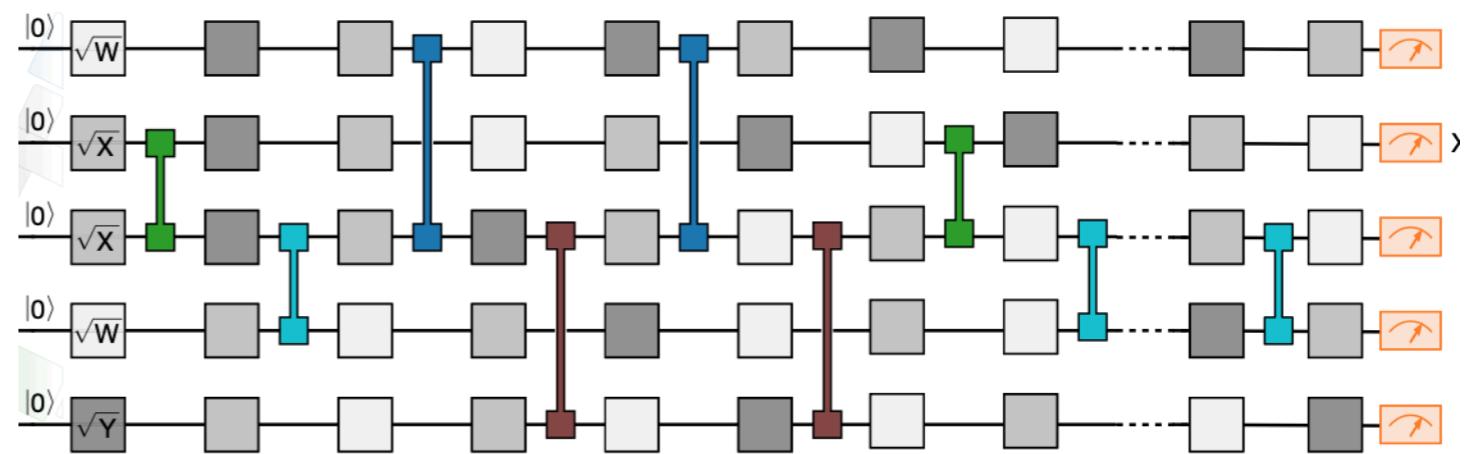
*Jordan-Wigner isomorphism - preserve the spectrum*

# Quantum Algorithms for NISQ era

NISQ: noisy intermediate-scale quantum computer



# qubits ~ 10 to 100



gate depth ~ 10 to 100

What are practical quantum algorithms for simulations on NISQ devices?

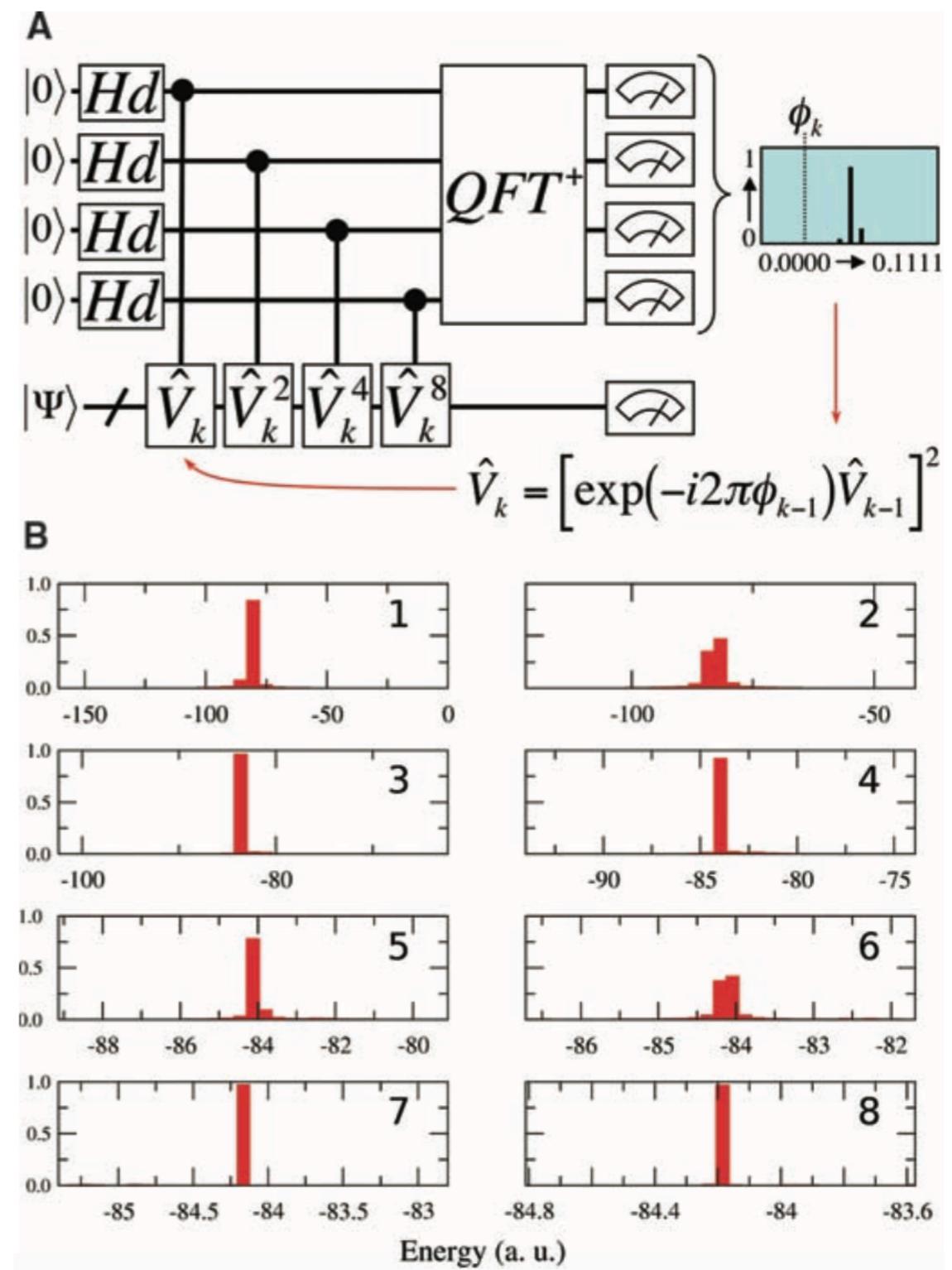
# Quantum Algorithms for NISQ era

## Phase Estimation<sup>1, 2</sup>

Perform the unitary quantum dynamics

$$e^{-2\pi i Hx} \quad x = 2^k$$

and measure the spectrum.<sup>3</sup>



<sup>1</sup> Kitaev, arXiv:quant-ph/9511026 (1995).

(Figure from ref 3)

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# Quantum Algorithms for NISQ era

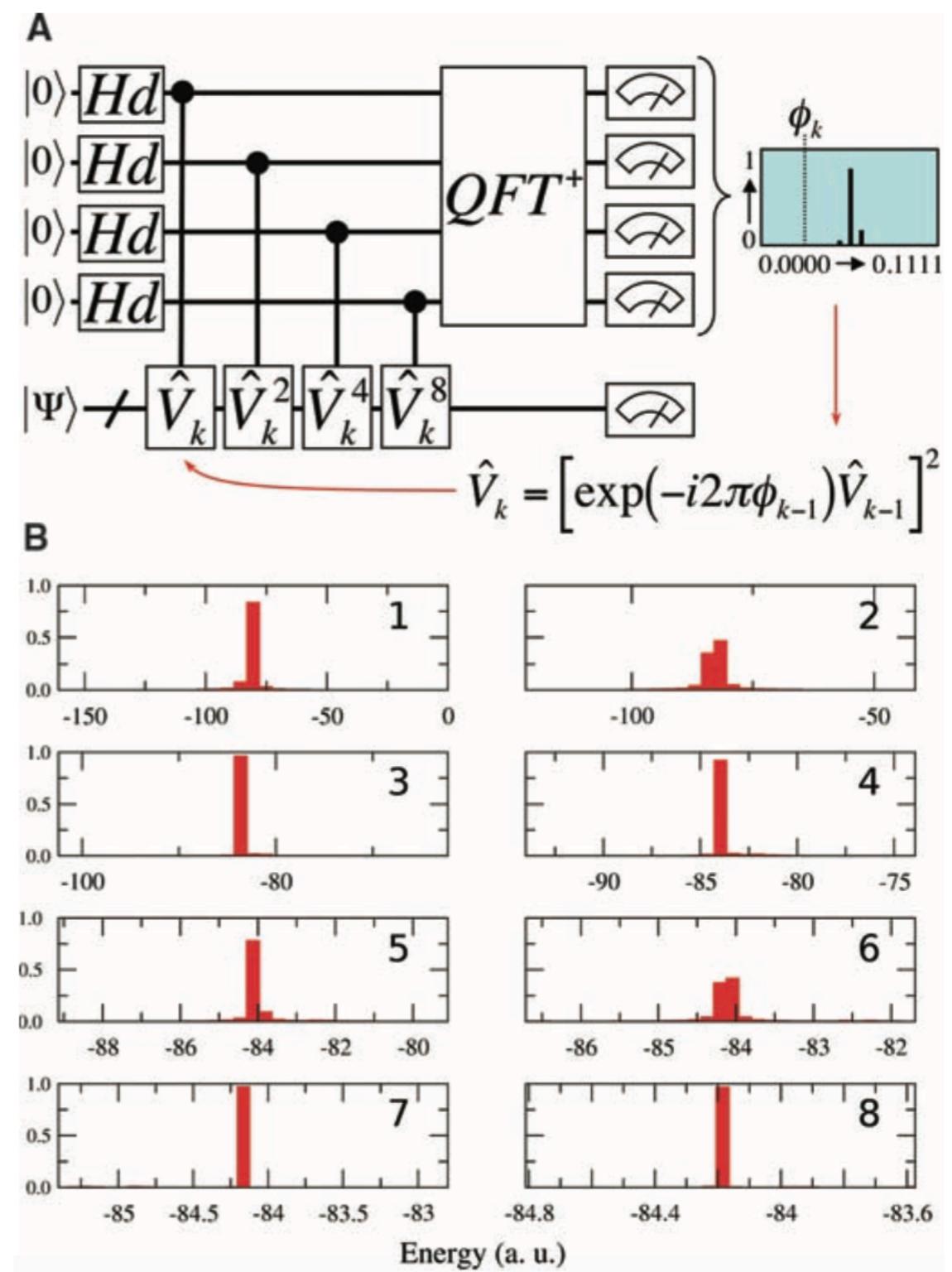
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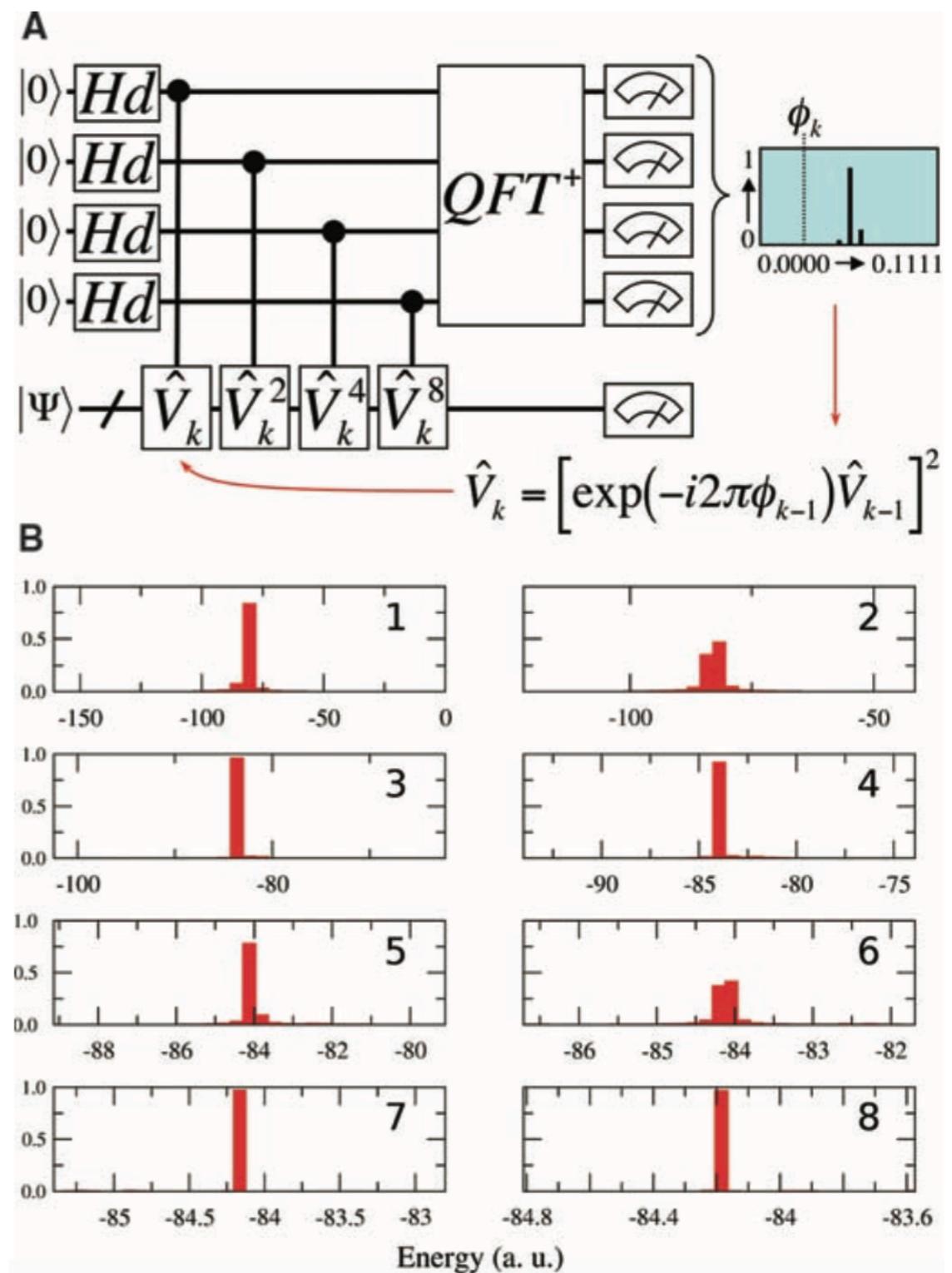
Perform the unitary quantum dynamics

$$e^{-2\pi i Hx} \quad x = 2^k$$

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- project to exact ground state and energy
- ancillary qubits
- many controlled gates → long circuits (need error correction)

**NOT suitable for NISQ era**



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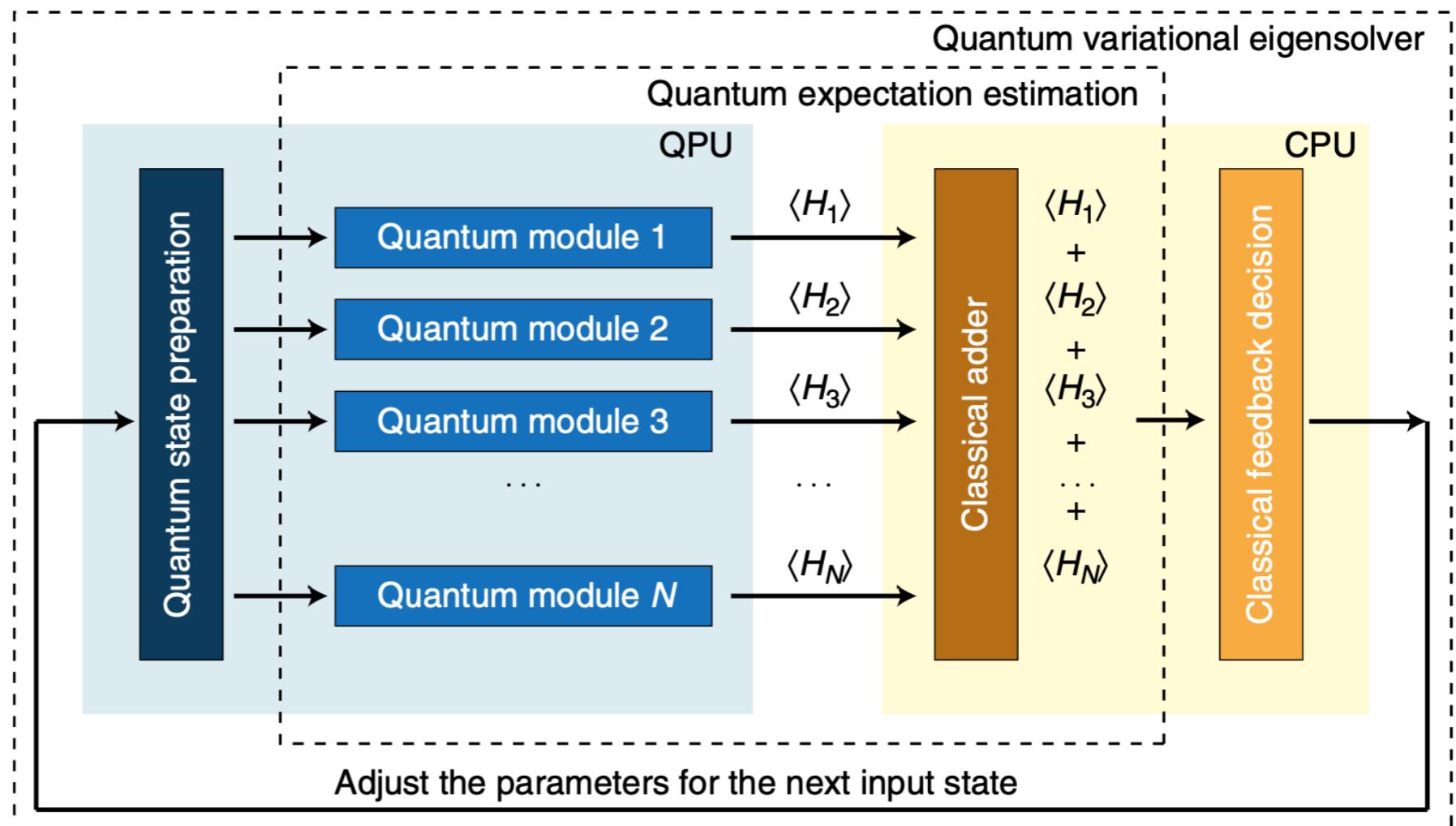
# Quantum Algorithms for NISQ era

## Variational Quantum Eigensolver (VQE)<sup>1-4</sup>

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

Prepare states on quantum computers

Optimize parameters variationally on classical computers



(Figure from ref 1)

- exploit shallow circuits

<sup>1</sup> Peruzzo, et al. *Nat. Commun.* (2014).

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<sup>4</sup> O'Malley, et al. *Phys. Rev. X* (2016).

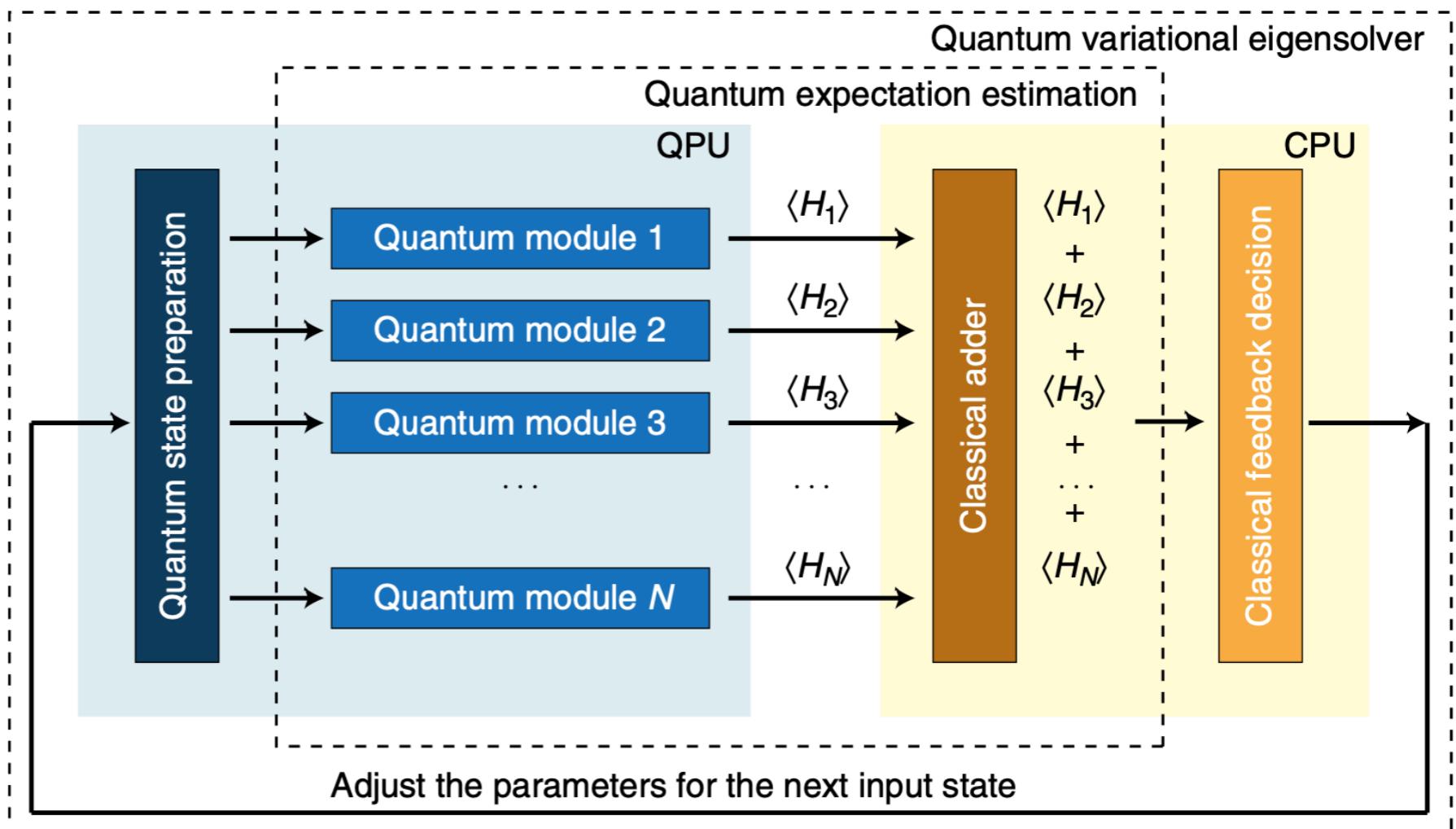
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(Figure from ref 1)

- exploit shallow circuits
- challenging high dimensional noisy classical optimization
- many measurements required for energy convergence

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# Quantum Algorithms for NISQ era

## Quantum Subspace Diagonalization (QSD)<sup>1-4</sup>

Prepare a set of **non-orthogonal** states on quantum computers (as basis)

$$|\psi_\alpha\rangle = \hat{U}_\alpha |\Phi_0\rangle, \quad \alpha = 1, \dots, N$$

Estimate overlap and Hamiltonian matrix elements from **measurements**

$$S_{\alpha\beta} = \langle\psi_\alpha|\psi_\beta\rangle \quad H_{\alpha\beta} = \langle\psi_\alpha|\hat{H}|\psi_\beta\rangle$$

Obtain energies by solving a generalized eigenvalue problem

$$\mathbf{H}\mathbf{C} = \mathbf{SCE}$$

- possible to avoid classical optimization
- excited states

<sup>1</sup> McClean, Kimchi-Schwartz, Carter, de Jong, *Phys. Rev. A* (2017). <sup>3</sup> Motta, et al. *Nat. Phys.* (2019).

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- possible to avoid classical optimization
- excited states
- How to measure matrix elements efficiently?
- How to mitigate numerical stability problem?

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# Multireference Selected Quantum Krylov (MRSQK)

Recent work explored the **Quantum Krylov subspace strategy**

**Quantum Lanczos  
(QLanczos)<sup>3</sup>**

imaginary-time grid basis  
non-unitary operation  
 $|\psi'\rangle = e^{-\tau\hat{H}}|\psi\rangle$

$\{|\Phi\rangle, e^{-2\Delta\tau H}|\Phi\rangle, e^{-4\Delta\tau H}|\Phi\rangle, \dots\}$

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**MRSQK,  
Quantum Filter  
Diagonalization** <sup>4</sup>

real-time grid basis  
 $|\psi(t)\rangle = e^{-it\hat{H}} |\psi(0)\rangle$

$$\{ |\Phi\rangle, e^{-i\Delta t \hat{H}} |\Phi\rangle, e^{-i2\Delta t \hat{H}} |\Phi\rangle, \dots \}$$

**natural on a quantum computer!**

<sup>1</sup> McClean, Kimchi-Schwartz, Carter, de Jong, *Phys. Rev. A* (2017). <sup>3</sup> Motta, et al. *Nat. Phys.* (2019).  
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How to fix **Numerical instabilities**

**Quantum Lanczos  
(QLanczos)** <sup>3</sup> keep the  $k$ -th time-evolved state iff  $|\langle \Phi_k | \Phi_{k-1} \rangle| < s$ , where  $s$  is a regularization parameter.

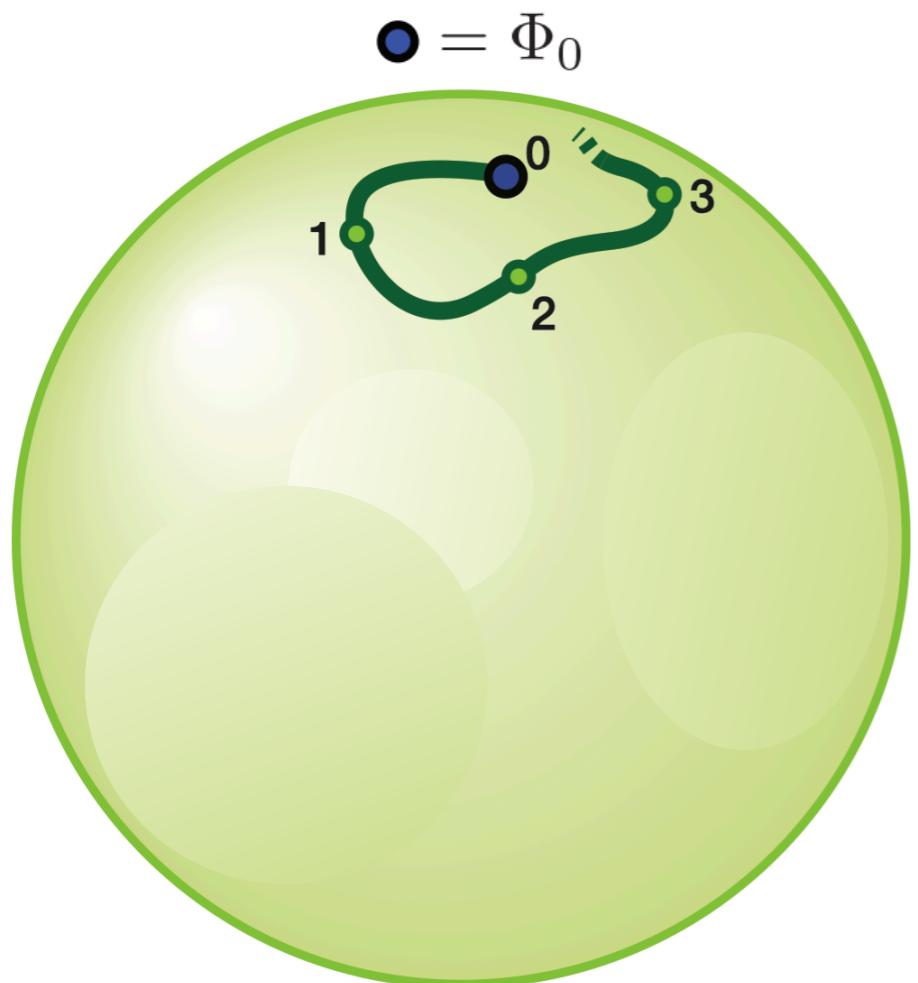
**MRSQK**

multireference real-time grid basis

<sup>1</sup> McClean, Kimchi-Schwartz, Carter, de Jong, *Phys. Rev. A* (2017). <sup>3</sup> Motta, et al. *Nat. Phys.* (2019).

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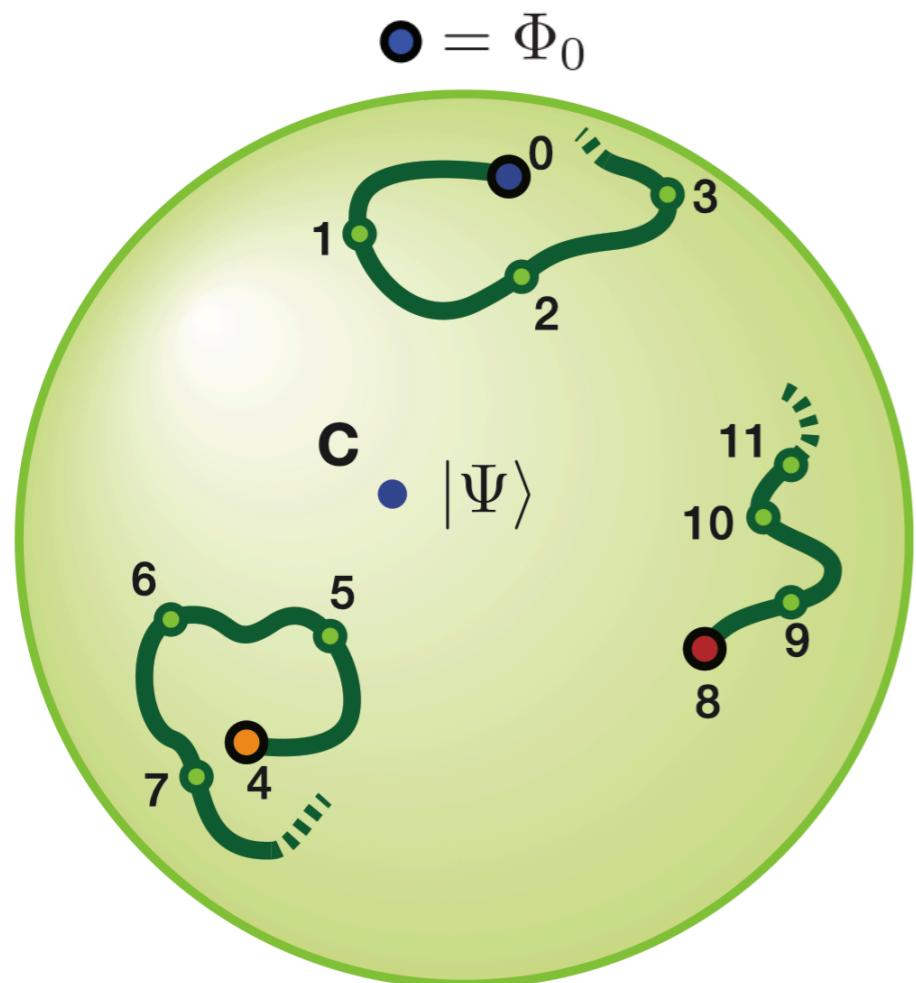
# Why we use multiple references in MRSQK?



$N$	$E_{\text{QK}}$	$k(\mathbf{S}_{\text{QK}})$
$\text{H}_6 (r_{\text{HH}} = 1.5 \text{ \AA})$		
4	-3.015510	$3.29 \times 10^5$
8	-3.019768	$3.60 \times 10^{11}$
12	-3.020172	$1.61 \times 10^{17}$
16	-3.020192	$3.19 \times 10^{17}$
20	-3.020198	$3.86 \times 10^{17}$
FCI	-3.020198	
$\text{H}_8 (r_{\text{HH}} = 1.5 \text{ \AA})$		
4	-4.017108	$1.19 \times 10^5$
8	-4.026563	$1.39 \times 10^{10}$
12	-4.028000	$5.11 \times 10^{14}$
16	-4.028096	$1.33 \times 10^{17}$
20	-	-
24	-	-
FCI	-4.028152	

time-evolved states from one reference determinant are linearly dependent.

# Why we use multiple references in MRSQK?

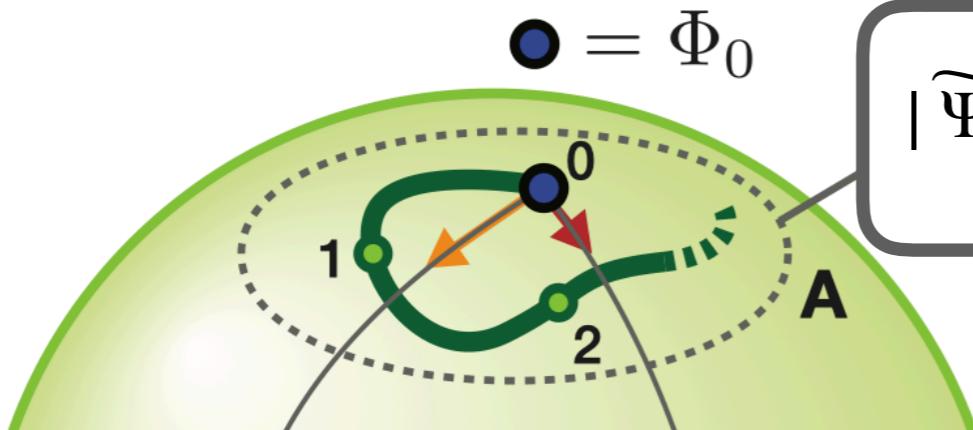


$N$	$E_{\text{QK}}$	$k(\mathbf{S}_{\text{QK}})$	$E_{\text{MRSQK}}$	$k(\mathbf{S}_{\text{MRSQK}})$
$\text{H}_6 (r_{\text{HH}} = 1.5 \text{ \AA})$				
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12	-3.020172	$1.61 \times 10^{17}$	-3.019696	$9.39 \times 10^5$
16	-3.020192	$3.19 \times 10^{17}$	-3.019835	$5.68 \times 10^6$
20	-3.020198	$3.86 \times 10^{17}$	-3.019929	$6.23 \times 10^6$
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4	-4.017108	$1.19 \times 10^5$	-4.017108	$1.19 \times 10^5$
8	-4.026563	$1.39 \times 10^{10}$	-4.024268	$1.50 \times 10^5$
12	-4.028000	$5.11 \times 10^{14}$	-4.025894	$2.00 \times 10^5$
16	-4.028096	$1.33 \times 10^{17}$	-4.026042	$2.51 \times 10^5$
20	-	-	-4.026387	$4.27 \times 10^5$
24	-	-	-4.026457	$4.44 \times 10^5$
FCI	-4.028152			

Multireference strategy can mitigate numerical instability

# How we select references?

1. Build a trial ground state  $|\tilde{\Psi}_0\rangle$

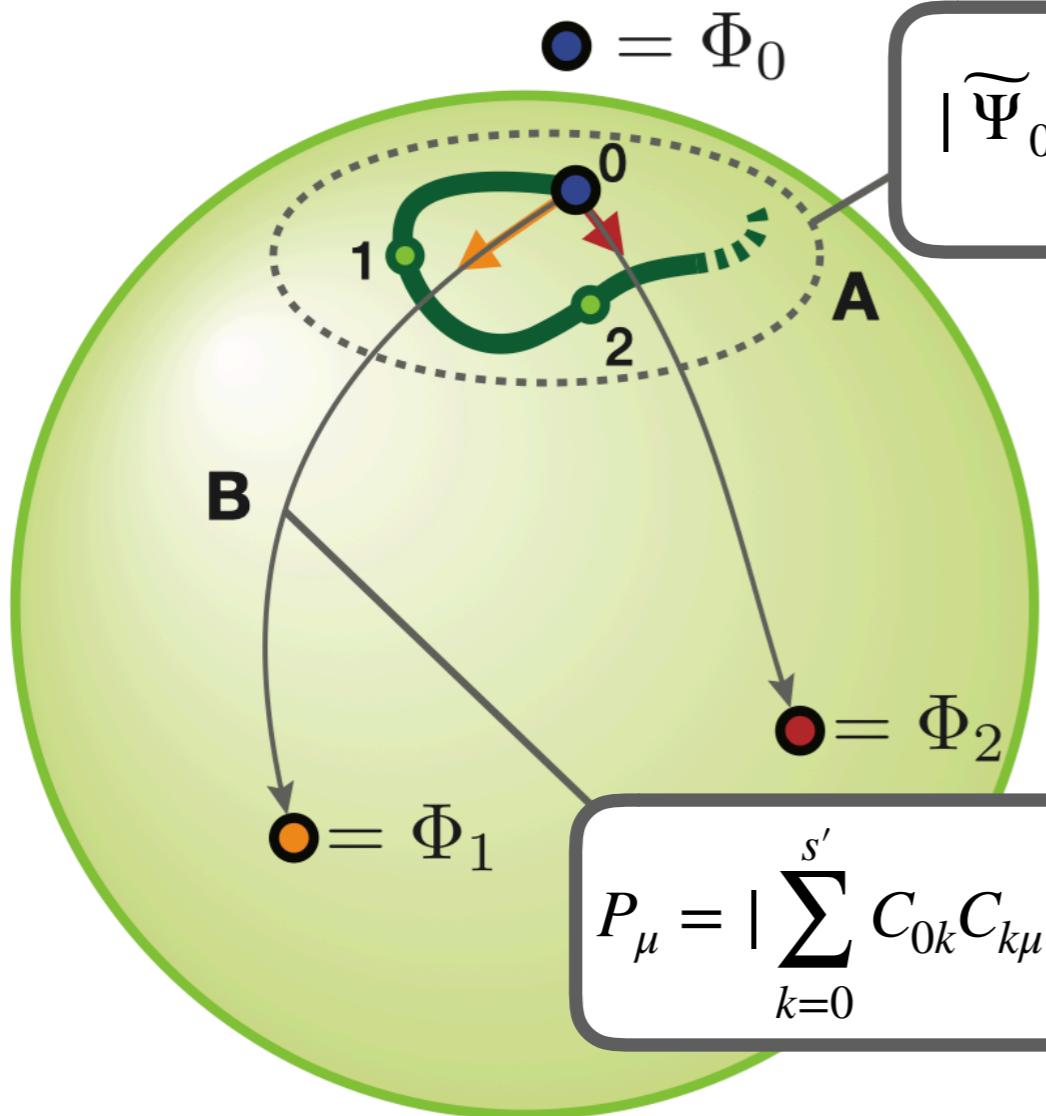


$$|\tilde{\Psi}_0\rangle = \sum_{k=0}^{s'} C_{0k} e^{-ik\Delta t \hat{H}} |\Phi_0\rangle = \sum_{k=0}^{s'} \sum_{\mu=0}^{2^n-1} C_{0k} C_{k\mu} |\mu\rangle$$

$\{|\mu\rangle\}$  - n-qubit computational basis states (determinants)

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{ $|\mu\rangle$ } - n-qubit computational basis states (determinants)

$$P_\mu = \left| \sum_{k=0}^{s'} C_{0k} C_{k\mu} \right|^2 \approx \sum_k \left| C_{0k} \right|^2 \left| C_{k\mu} \right|^2$$

2. Use direct measurements to get the probability of sampling  $|\mu\rangle$  in  $|\tilde{\Psi}_0\rangle$

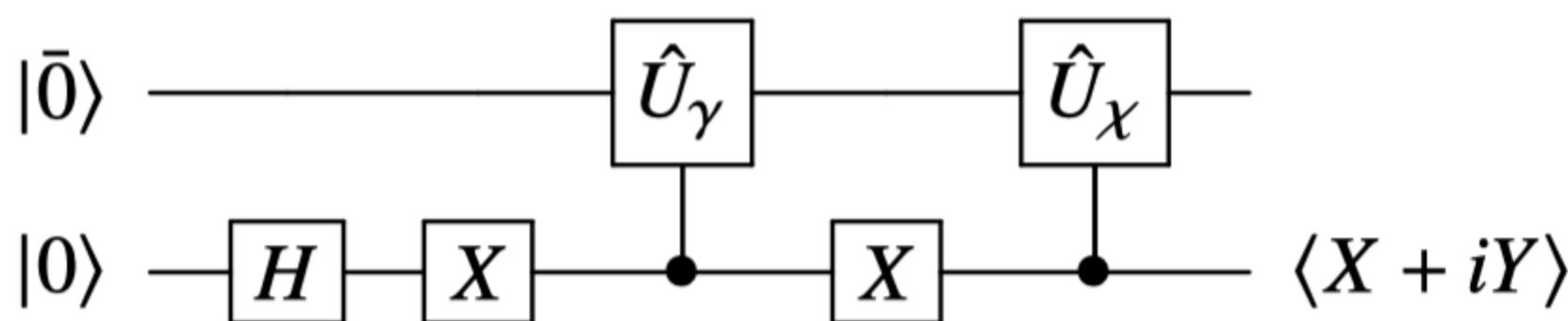
# How we measure matrix elements?

- matrix elements in MRSQK:

$$S_{\alpha\beta} = \langle \psi_\alpha | \psi_\beta \rangle = \langle \Phi_I | \hat{U}_m^\dagger \hat{U}_n | \Phi_J \rangle$$

$$H_{\alpha\beta} = \langle \psi_\alpha | \hat{H} | \psi_\beta \rangle = \langle \Phi_I | \hat{U}_m^\dagger \hat{H} \hat{U}_n | \Phi_J \rangle$$

- Hadamard test circuit for estimating  $\langle \bar{0} | \hat{U}_\gamma^\dagger \hat{U}_\chi | \bar{0} \rangle$



# How to implement the real-time dynamics? $e^{it\hat{H}}$

$$\hat{H} = \sum_l^N h_l \bigotimes_{k=1}^{n_l} \sigma_{l_k}^{\{X,Y,Z\}} = \sum_l^N h_l U_l$$

First-order Lie-Trotter-Suzuki product with  $m$  Trotter steps (numbers)

$$e^{-it\hat{H}} = \left( \prod_l^N e^{-i\delta_t \hat{U}_l} \right)^m + O(\delta_t),^1 \quad \delta_t = \frac{th_l}{m}$$

$$e^{-i\delta_t U_1} e^{-i\delta_t U_2} \dots e^{-i\delta_t U_N} \approx e^{-i\delta_t (\hat{H} + \Delta)},^2 \quad \Delta = i \sum_{j>k} [U_j, U_k] \frac{\delta_t}{2}$$

Errors of the product formula:

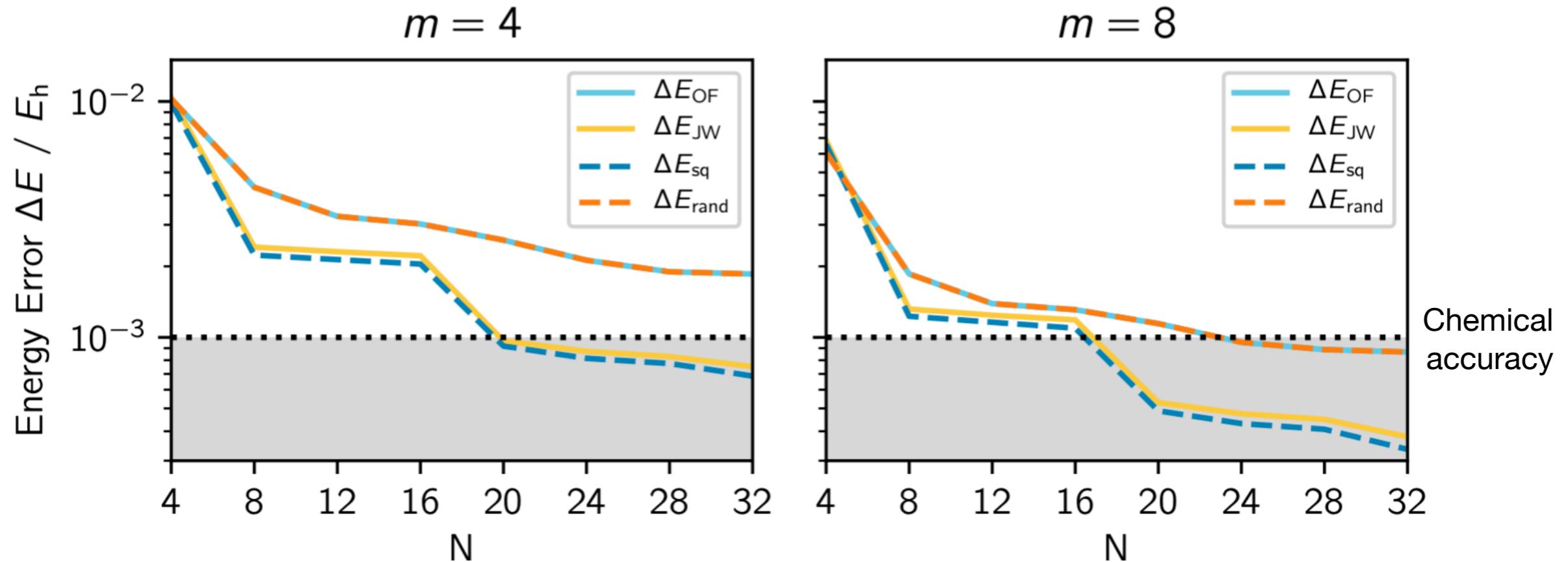
- Trotter number (number of Trotter step)  $m$
- Ordering of  $e^{-i\delta_t U_i}$  operators

<sup>1</sup> McArdle, Endo, Aspuru-Guzik, Yuan, Benjamin, arXiv:1808.10402 (2019).

<sup>2</sup> Hastings, Wecker, Bauer, Troyer, Quantum Inf. Comput. (2015).

# Is the product approximation good for MRSQK?

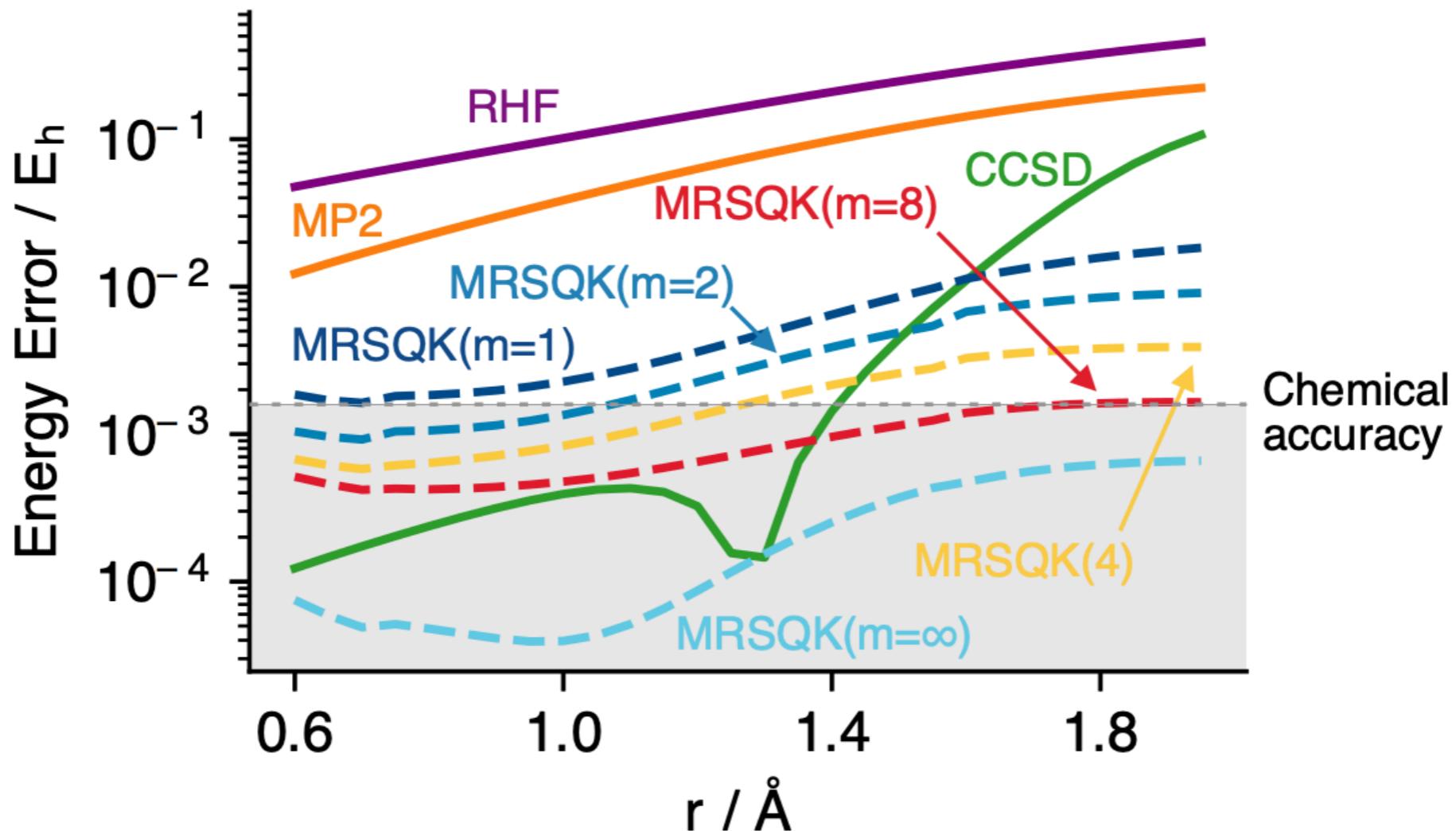
MRSQK results for linear  $\text{H}_6$   $\Delta E - N$  plot at bond length  $1.5\text{\AA}$



- MRSQK can achieve chemical accuracy using small Trotter number  $m$ .
- Different operator orderings have different energy convergence patterns.

# Is the product approximation good for MRSQK?

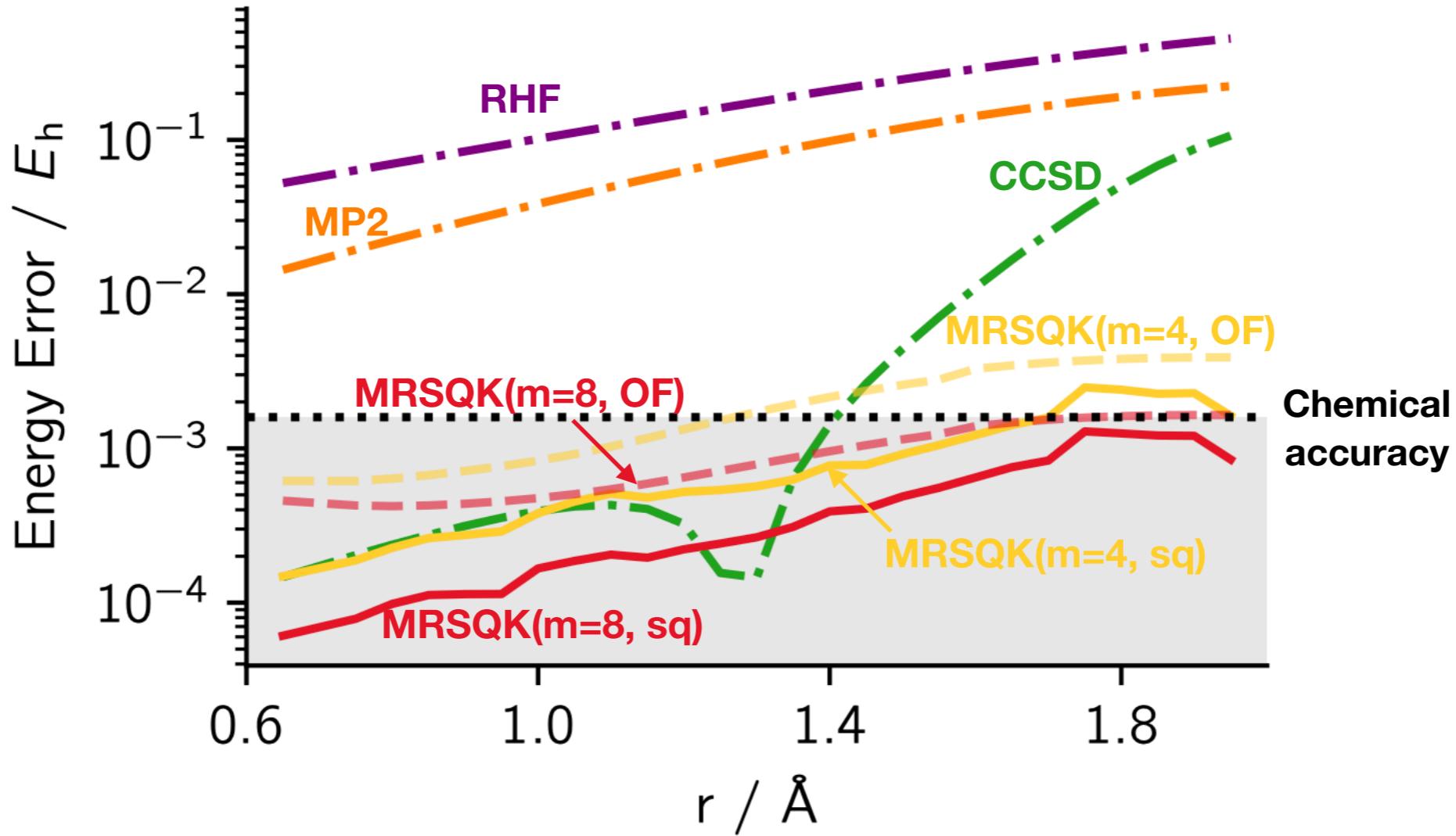
Potential energy curve for linear  $\text{H}_6$ , MRSQK using OF operator ordering



- MRSQK performs better than CCSD for large bond distance (over 1.6 Å) even with the lowest Trotter number  $m = 1$

# Is the product approximation good for MRSQK?

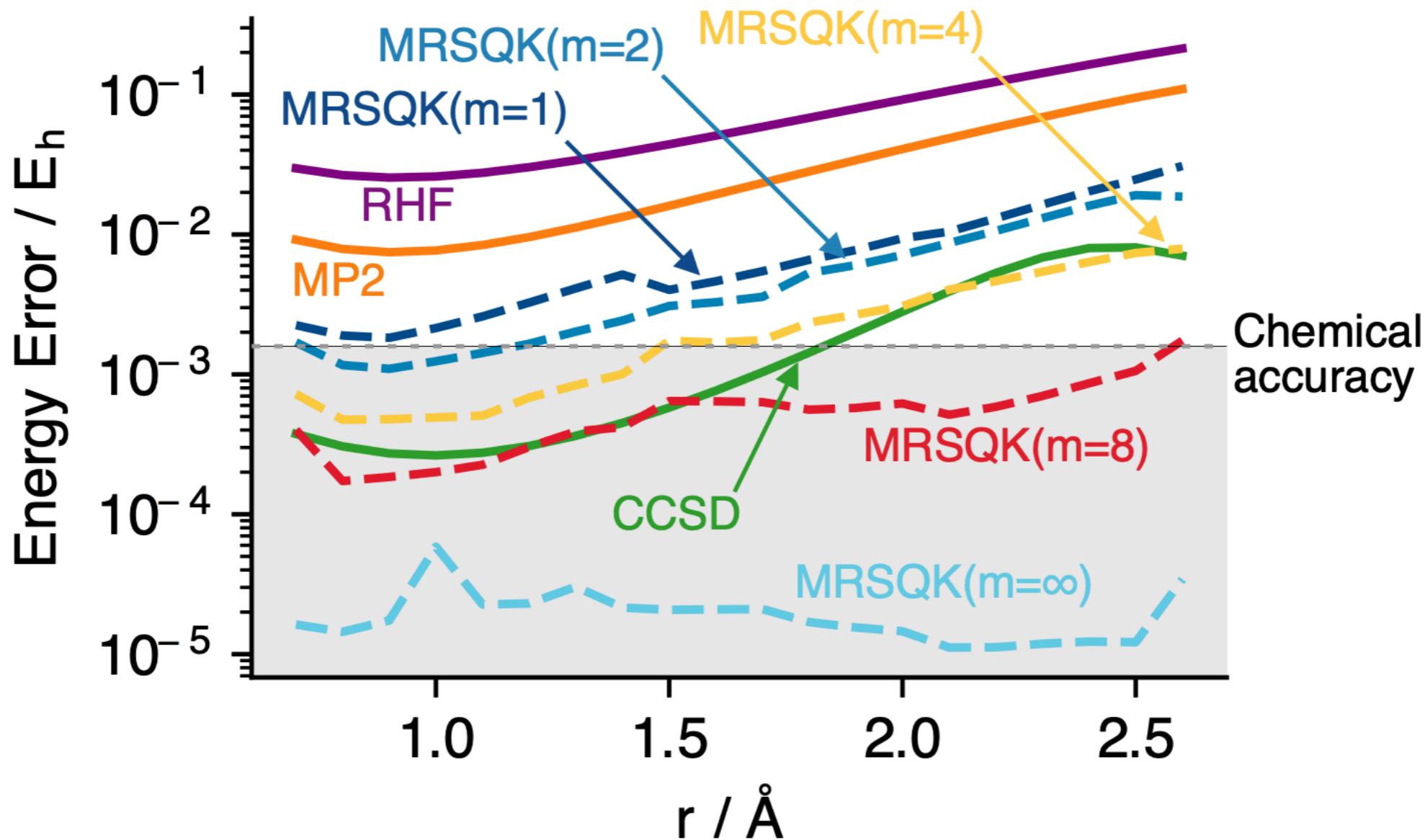
Potential energy curve for linear  $\text{H}_6$ , MRSQK using OF and sq operator ordering



- **MRSQK with  $m = 4$  and sq ordering** already achieves the same level of accuracy as CCSD at short bond distance range ( $0.6\text{\AA}$  to  $1.1\text{\AA}$ ), and better than CCSD for distances larger than  $1.4\text{\AA}$ .

# Is the product approximation good for MRSQK?

Potential energy curve for  $\text{BeH}_2$ , MRSQK using OF operator ordering



- MRSQK performs better than CCSD throughout the curve when  $m = 8$

# Conclusions

- **MRSQK is a new quantum algorithm for molecular simulation based on the real-time dynamics without classical optimization.**
- **MRSQK uses multiple references to mitigate numerical instability.**
- **Chemical accuracy can be achieved even with small Trotter number.**
- **Operator ordering is relevant to energy convergence.**

# Future work

## - MRSQK for excited states

MRSQK with 32 Krylov basis states and a large Trotter number  $m=100$  still gives an error of 5.1 mEh.

Table 3: First excited-state energies (in  $E_h$ ) of linear **H<sub>6</sub>** at a bond distance of 1.5 Å. MRSQK results are given for  $N = d(s+1)$  Krylov basis states using three steps ( $s = 3$ ) and  $\Delta t = 0.5$  a.u. Notations are consistent with those in Table 2.

$N$	$E_{\text{OF}}^{(m=2)}$	$E_{\text{JW}}^{(m=2)}$	$E_{\text{sq}}^{(m=2)}$	$E_{\text{rand}}^{(m=2)}$	$E_{\text{OF}}^{(m=4)}$	$E_{\text{JW}}^{(m=4)}$	$E_{\text{sq}}^{(m=4)}$	$E_{\text{rand}}^{(m=4)}$
8	-2.813678	-2.822952	-2.819339	-2.813678	-2.854913	-2.851219	-2.850036	-2.854913
16	-2.822238	-2.847035	-2.842780	-2.822238	-2.859053	-2.867098	-2.865905	-2.859053
24	-2.831772	-2.854135	-2.849167	-2.831772	-2.866840	-2.874047	-2.872074	-2.866840
32	-2.844701	-2.860495	-2.856910	-2.844701	-2.870509	-2.878594	-2.877274	-2.870509
$N$	$E_{\text{OF}}^{(m=8)}$	$E_{\text{JW}}^{(m=8)}$	$E_{\text{sq}}^{(m=8)}$	$E_{\text{rand}}^{(m=8)}$	$E_{\text{OF}}^{(m=100)}$	$E_{\text{JW}}^{(m=100)}$	$E_{\text{sq}}^{(m=100)}$	$E_{\text{rand}}^{(m=100)}$
8	-2.865878	-2.862217	-2.861961	-2.865878	-2.868958	-2.868574	-2.868583	-2.868958
16	-2.870392	-2.873199	-2.873127	-2.870392	-2.874589	-2.876091	-2.876461	-2.874589
24	-2.877971	-2.879774	-2.879015	-2.877971	-2.882155	-2.882154	-2.882124	-2.882155
32	-2.880205	-2.883214	-2.882670	-2.880205	-2.884504	-2.884840	-2.884817	-2.884504
FCI	-2.889922							

# Future work

- Reduce gate counts and circuit depth

Table 1: Resource estimates for MRSQK calculations with  $m = 1$  Trotter step approximation on several hydrogen systems in STO-6G basis at the bond length  $R=1.5 \text{ \AA}$ . Jordan-Wigner transformation is used to encode the Hamiltonian for all cases in the table.

	H <sub>2</sub>	H <sub>4</sub> (linear)	H <sub>4</sub> (ring)	H <sub>6</sub> (linear)	H <sub>6</sub> (ring)	H <sub>8</sub> (linear)
Num. of qubits	4	8	8	12	12	16
Num. of Pauli terms	14	184	92	918	702	2912
Num. of $H/R_{zy}$ ( $H_k$ ) gates	16	480	224	2832	2240	9664
Num. of 1-qubit gate layers	8	296	112	1680	1248	5552
Num. of CNOT gates	36	1328	520	9972	7476	41600
Num. of c- $R_z$ gates	14	184	92	918	702	2912
Num. of total layers	58	1808	724	12570	9426	50064

$$\bar{N}_{1-q} = m \sum_l^N 2w_l$$

$$\bar{N}_{\text{CNOT}} = m \sum_l^N 2(w_l - 1)$$

$$\bar{N}_{R_2} = Nm$$

$$\bar{N}_{\text{layer}} = m \sum_l^N (2w_l + 2\delta_l^Z - 1)$$

# Acknowledgements

## The group



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## QCQC Project Collaborators



## Funding



## Software



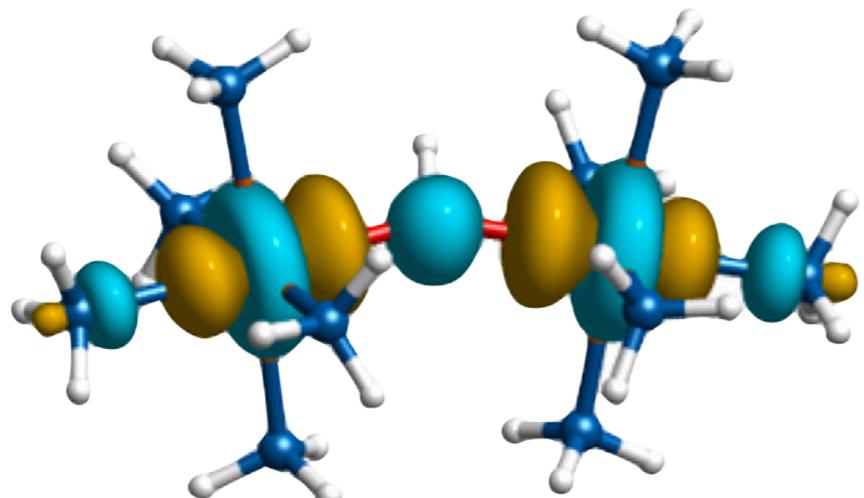
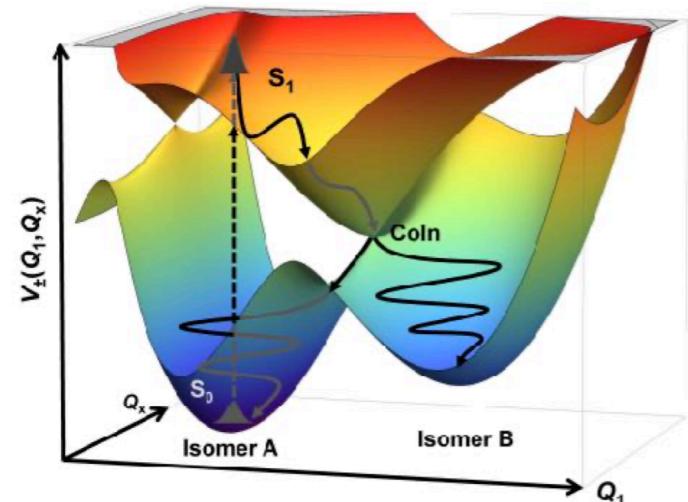
Thank You for Your Attention!



# Supplementary

## Why we want to develop quantum algorithms for chemistry problems?

**Strong/static correlation is important in quantum chemistry, and challenging for classical methods.**

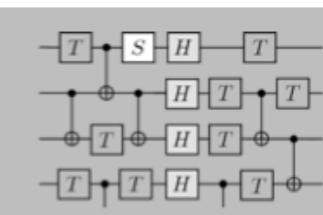


**Achieving useful applications and building full-stack quantum computer systems will hasten their development and potential for scientific discovery.**

### Quantum Computer Stack

#### Algorithms

Identify problem  
Map to qubits and gates



#### Quantum Software

Express in native gates/connectivity  
Compile & compress circuits  
Deploy error correction strategy



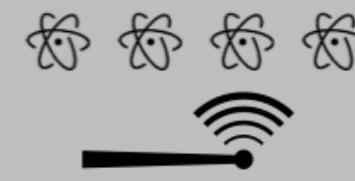
#### Control Engineering

Implement Hamiltonian control with E/M fields

$$i\hbar \frac{\partial |\Psi\rangle}{\partial t} = H(t)|\Psi\rangle$$

#### Qubit Technology

Interface control fields with qubit system



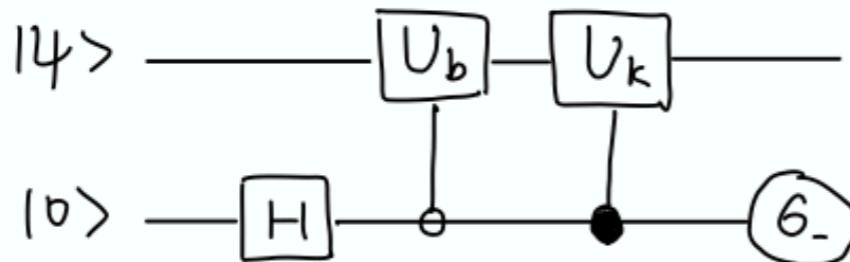
# Supplementary

**For small  $\Delta t$ , basis generated by real-time evolution spans a classical Krylov space**

$$\begin{aligned} |\Psi\rangle &= \sum_{n=0}^s c_I^{(n)} e^{-in\Delta t \hat{H}} |\Phi_I\rangle \\ &= \sum_{k=0}^s \left( \sum_{n=0}^s \frac{(-in\Delta t)^k}{k!} c_I^{(n)} \right) \hat{H}^k |\Phi_I\rangle + O(\Delta t^{s+1}) \\ &= \sum_{k=0}^s \left( \sum_{n=0}^s M_{kn} c_I^{(n)} \right) \hat{H}^k |\Phi_I\rangle + O(\Delta t^{s+1}) \end{aligned}$$

# Supplementary

## Hadamard test



$X \otimes I$

$$\frac{|0\rangle + |1\rangle}{\sqrt{2}}|4\rangle$$

$$|\psi_i\rangle = |0\rangle|4\rangle$$

$$\frac{|0\rangle|U_b|4\rangle + |1\rangle|4\rangle}{\sqrt{2}}$$

$$(|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U_k)(|0\rangle\langle 0| \otimes U_b + |1\rangle\langle 1| \otimes I)(H \otimes I)|0\rangle|4\rangle$$

$$= (|0\rangle\langle 0| H \otimes U_b + |1\rangle\langle 1| H \otimes U_k)|0\rangle|4\rangle \underset{(X \otimes I)}{\frac{|0\rangle|4\rangle + |1\rangle|U_b|4\rangle}{\sqrt{2}}}$$

$$= \frac{1}{\sqrt{2}}|0\rangle \otimes U_b|4\rangle + \frac{1}{\sqrt{2}}|1\rangle \otimes U_k|4\rangle$$

$$= |\psi_f\rangle$$

$$= \frac{|1\rangle|4\rangle + |0\rangle|U_b|4\rangle}{\sqrt{2}}$$

$$\langle \psi_f | 6_- \otimes I | \psi_f \rangle$$

$$6_- = \frac{x+iy}{2} = |0\rangle\langle 1|$$

$$= \frac{1}{2} (\langle 0| \otimes \langle 4| U_b^\dagger + \langle 1| \otimes \langle 4| U_k^\dagger) (|0\rangle\langle 1| \otimes I)$$

$$(|0\rangle \otimes U_b|4\rangle + |1\rangle \otimes U_k|4\rangle)$$

$$= \frac{1}{2} \langle 4| U_b^\dagger U_k |4\rangle$$