Measurement-Driven Quantum Algorithms

Efficient Eigensolvers and Evaluation of Matrix Functions

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IPAM Workshop: Bridging the Gap Between NISQ and FTQC

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ODMD

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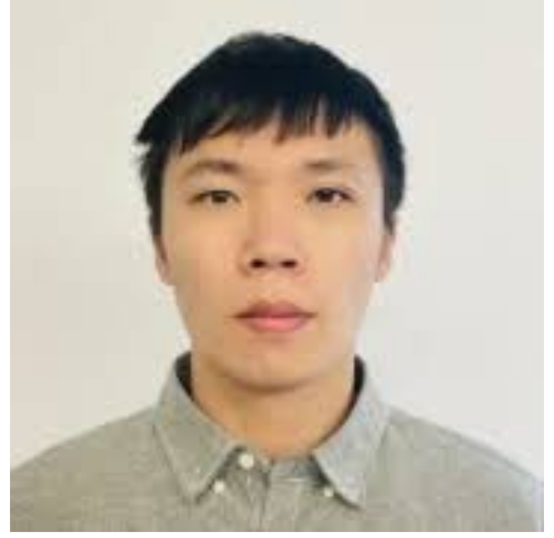
arXiv:2306.01858

ODMD



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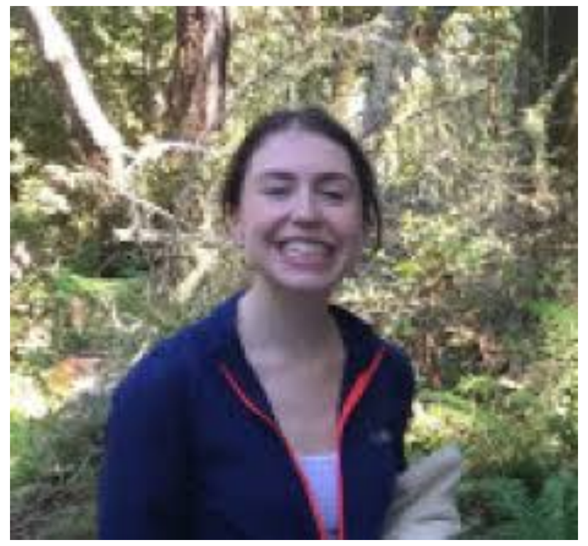

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Susanne Yelin (Harvard)

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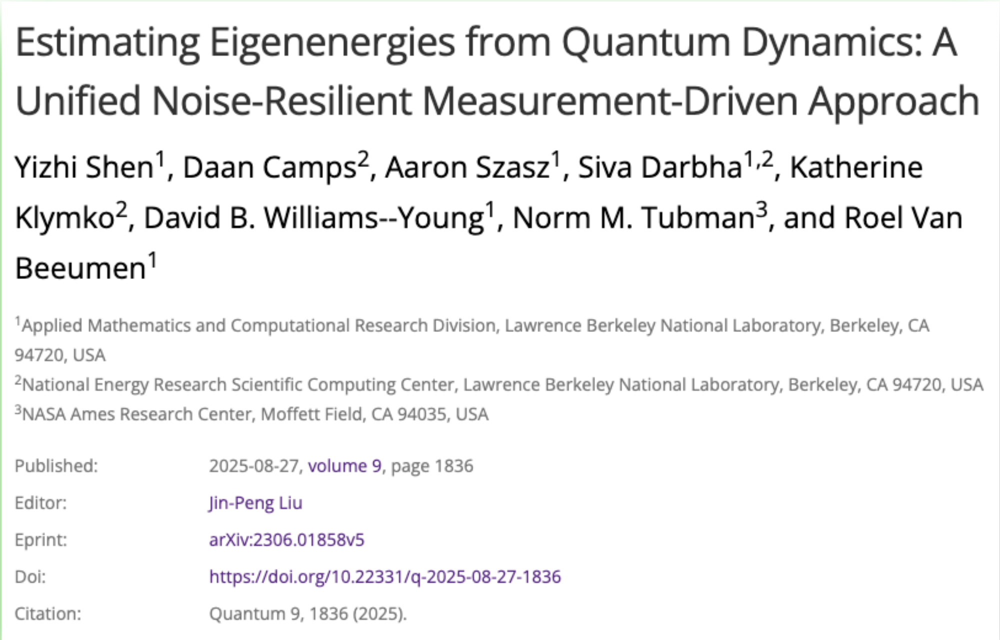
MODMD



Estimating Eigenenergies from Quantum Dynamics: A Unified Noise-Resilient Measurement-Driven Approach

Yizhi Shen[1], Daan Camps[2], Aaron Szasz[1], Siva Darbha[1,2], Katherine Klymko[2], David B. Williams--Young[1], Norm M. Tubman[3], and Roel Van Beeumen[1]

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SZEGÖ

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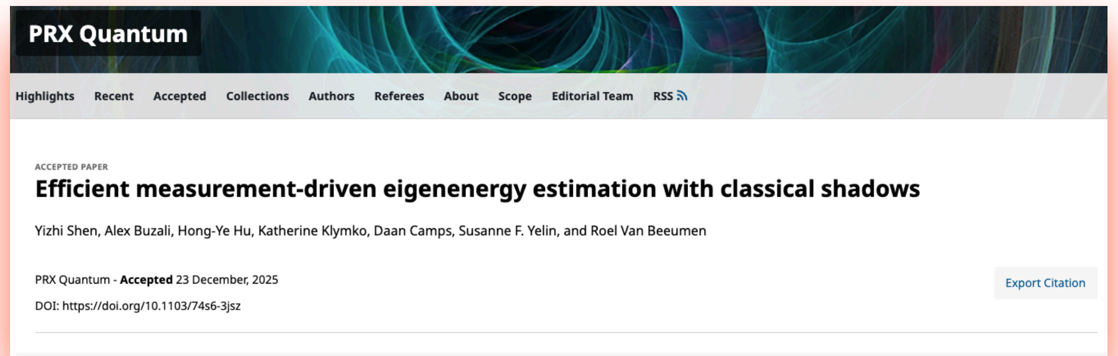

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ACCEPTED PAPER

Efficient measurement-driven eigenenergy estimation with classical shadows

Yizhi Shen, Alex Buzali, Hong-Ye Hu, Katherine Klymko, Daan Camps, Susanne F. Yelin, and Roel Van Beeumen

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Quantum Physics

[Submitted on 23 Sep 2025]

Quantum Krylov Algorithm for Szegö Quadrature

Introduction

NISQ vs (e)FTQC

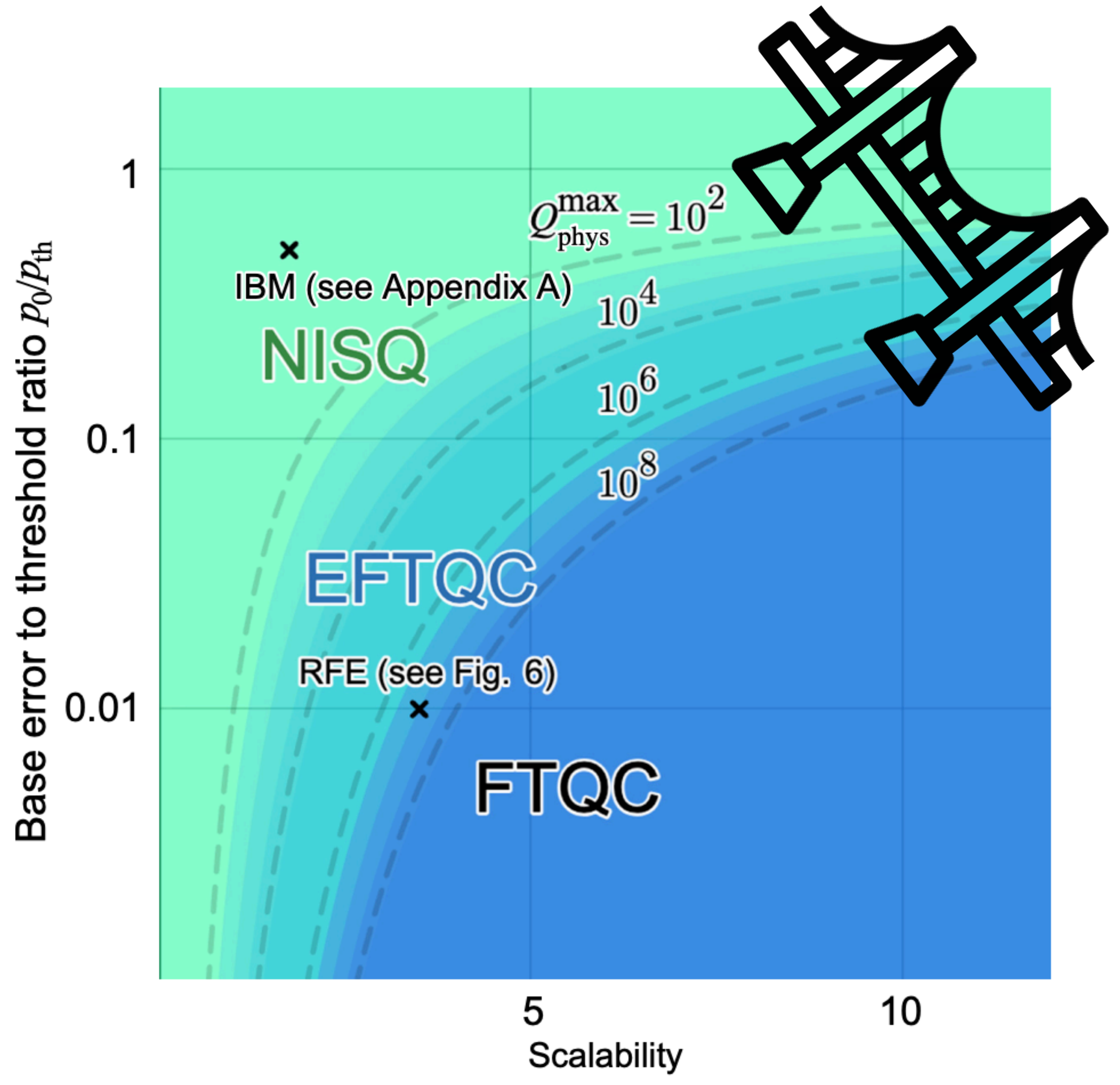
An algorithm developers POV

?

	NISQ	(e)FTQC
Circuit	• Optimize CNOT count • Optimize #qubits • Optimize for QPU connectivity	• Optimize T count or depth • Optimize #qubits • Optimize routing, moves etc • Optimize QEC codes
Algorithm	• Variational Quantum Eigensolver (VQE) • Quantum Approximate Optimization Algorithm (QAOA) • ...	• Quantum Phase Estimation (QPE) • Qubitization • Quantum Signal Processing (QSP) • ...
Performance metrics	• Improve convergence • Solution quality	

Measurement-Driven Approaches?

An Architecture POV



[Katabarwa, Gratsea, Caesura, Johnson 2024]

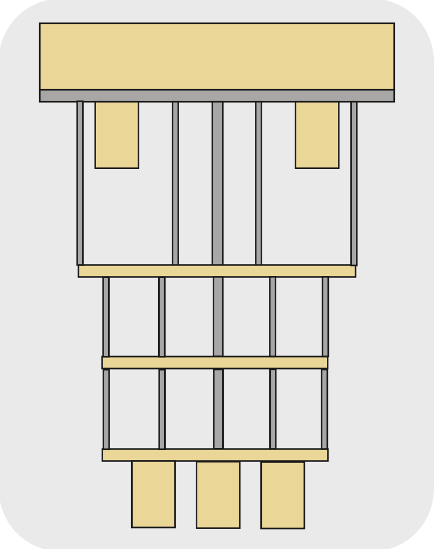
Errors + Scalability?

Measurement-Driven Approaches

A possible way to bridge the gap?

Unitary circuit, often time evolution

Run Quantum Circuit



Add Measurement Results

010…010
111…001
100…101
…

Postprocess

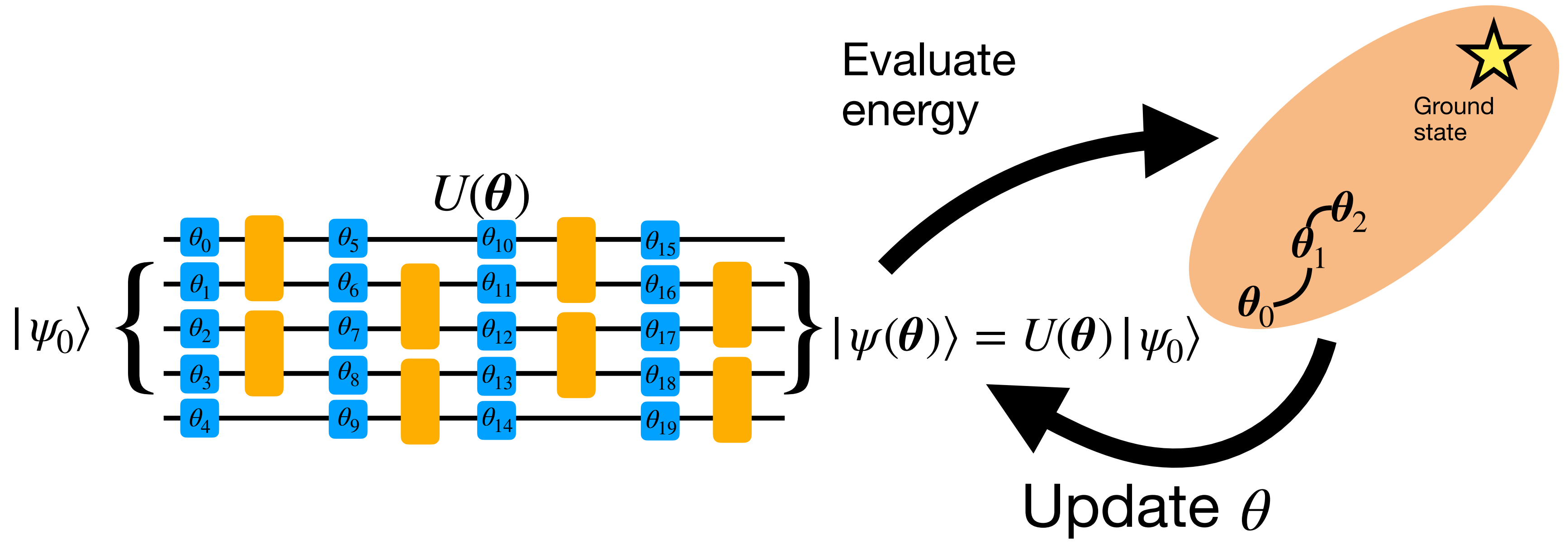
Based on classical methods in signal processing and linear algebra

(Repeat to improve results)

Running more circuits:

- grows the data set, improves the result
- typically does not require variational parameter updates in the circuit

Parametrized Quantum Circuits



Updates $\boldsymbol{\theta}$ but may get stuck

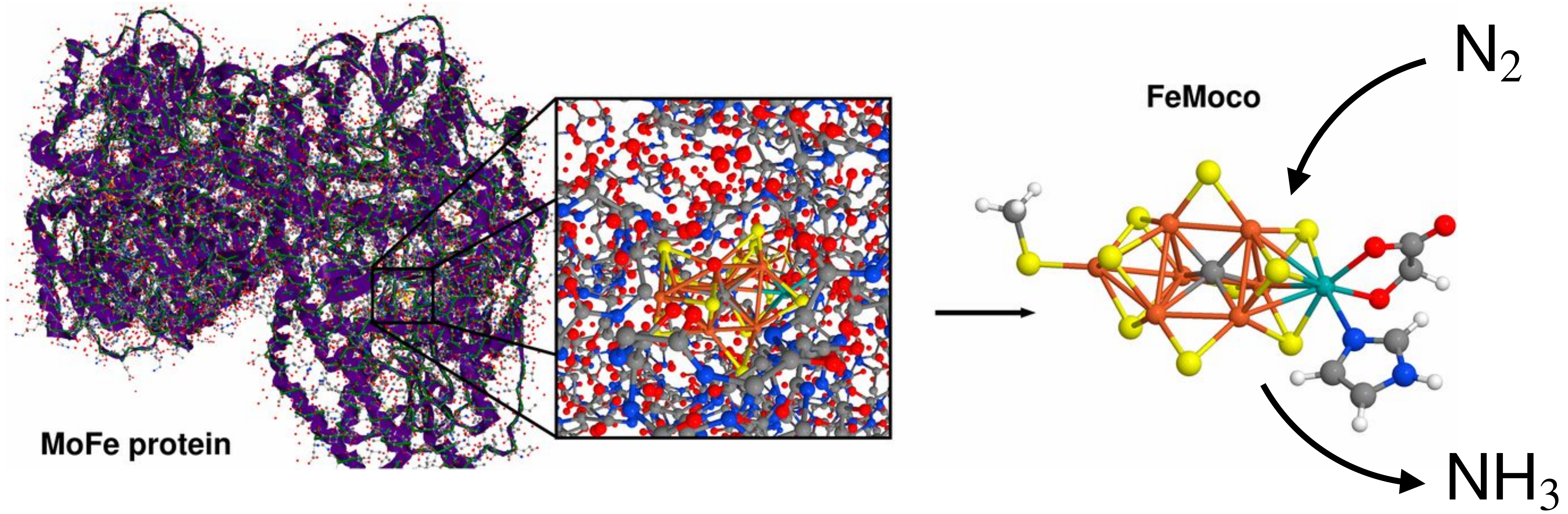
[Larocca, Thanasilp, Wang et al. 2025]

Part I. Estimating Eigenenergies.

Problem formulation

Computing select low-lying eigenenergies and states

How to efficiently estimate **low-lying eigenvalues** of a many-body **Hamiltonian?**



[Reiher, Wiebe, Svore et al. 2017]

Detailed understanding and prediction of molecular processes requires **high-precision energy** calculations

[Submitted on 8 Jan 2026]

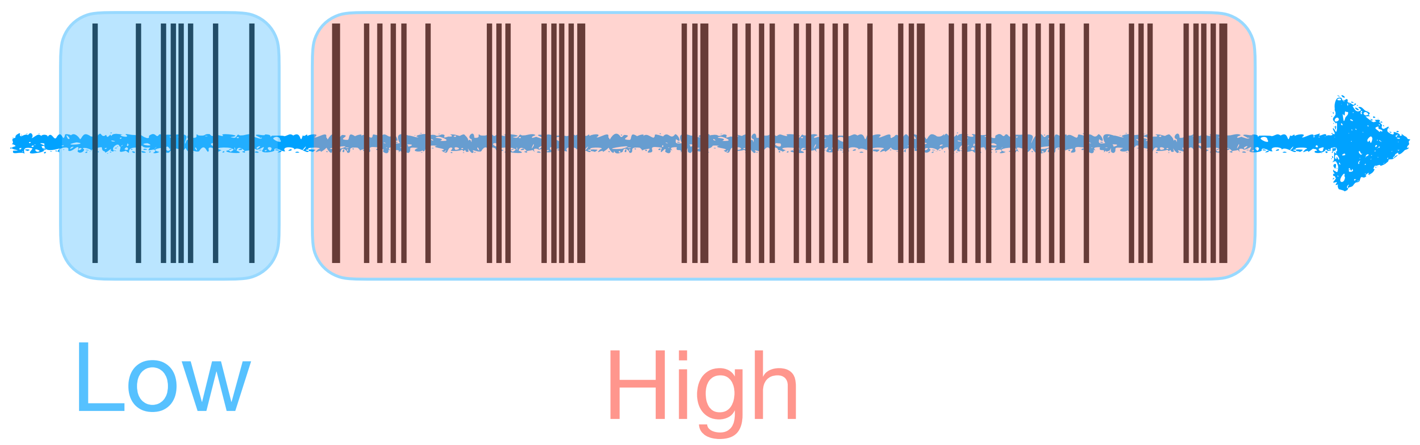
Classical solution of the FeMo-cofactor model to chemical accuracy and its implications

Huanchen Zhai, Chenghan Li, Xing Zhang, Zhendong Li, Seunghoon Lee, Garnet Kin-Lic Chan

Large eigenvalue problem

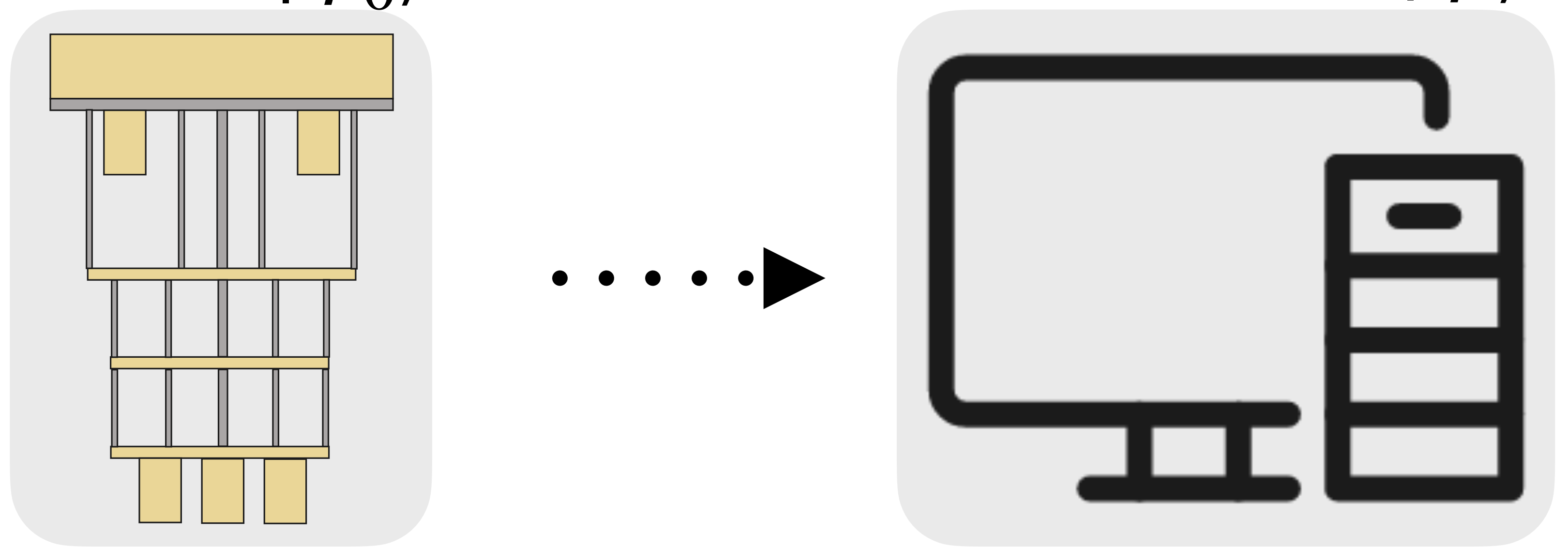
$$H\,|\,\phi\rangle = E\,|\,\phi\rangle$$

Energy spectrum



Query U that encodes H, $|\psi_0\rangle$

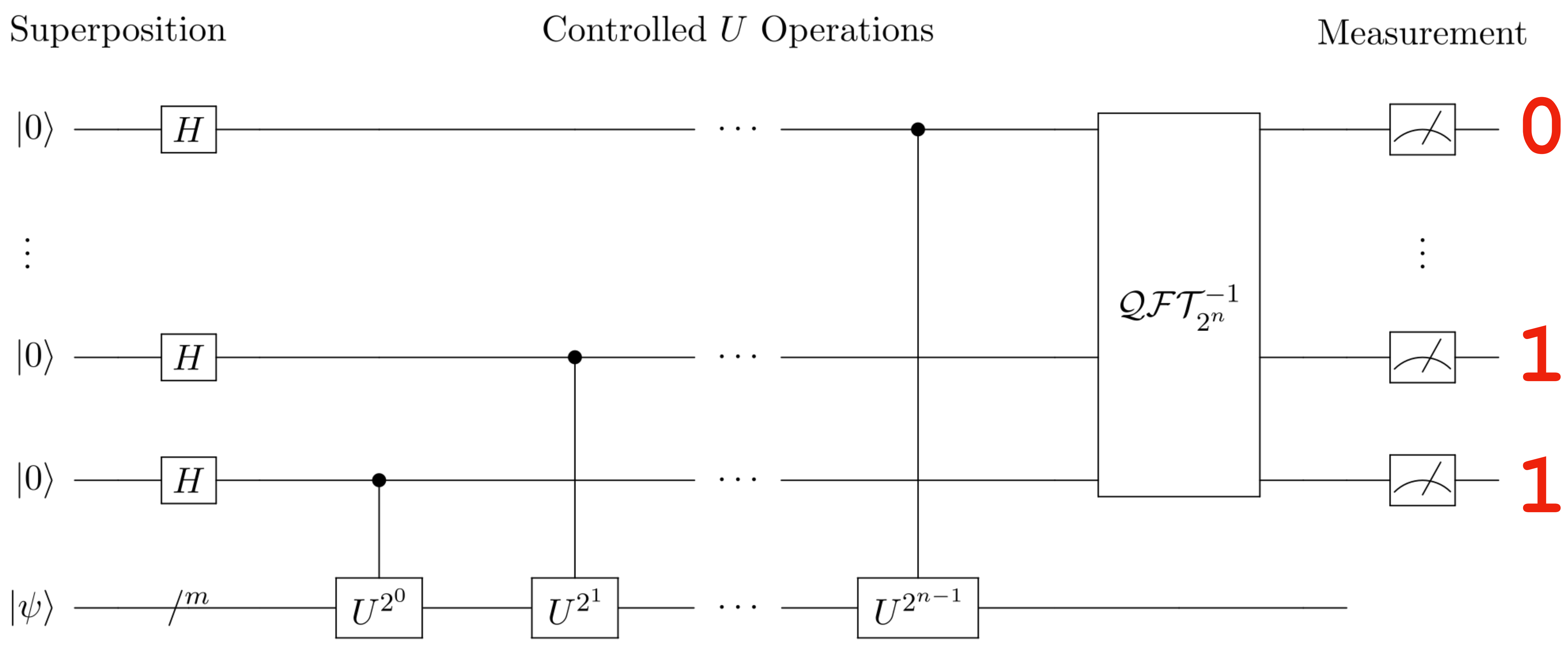
Estimates for E, (properties of) $|\phi\rangle$

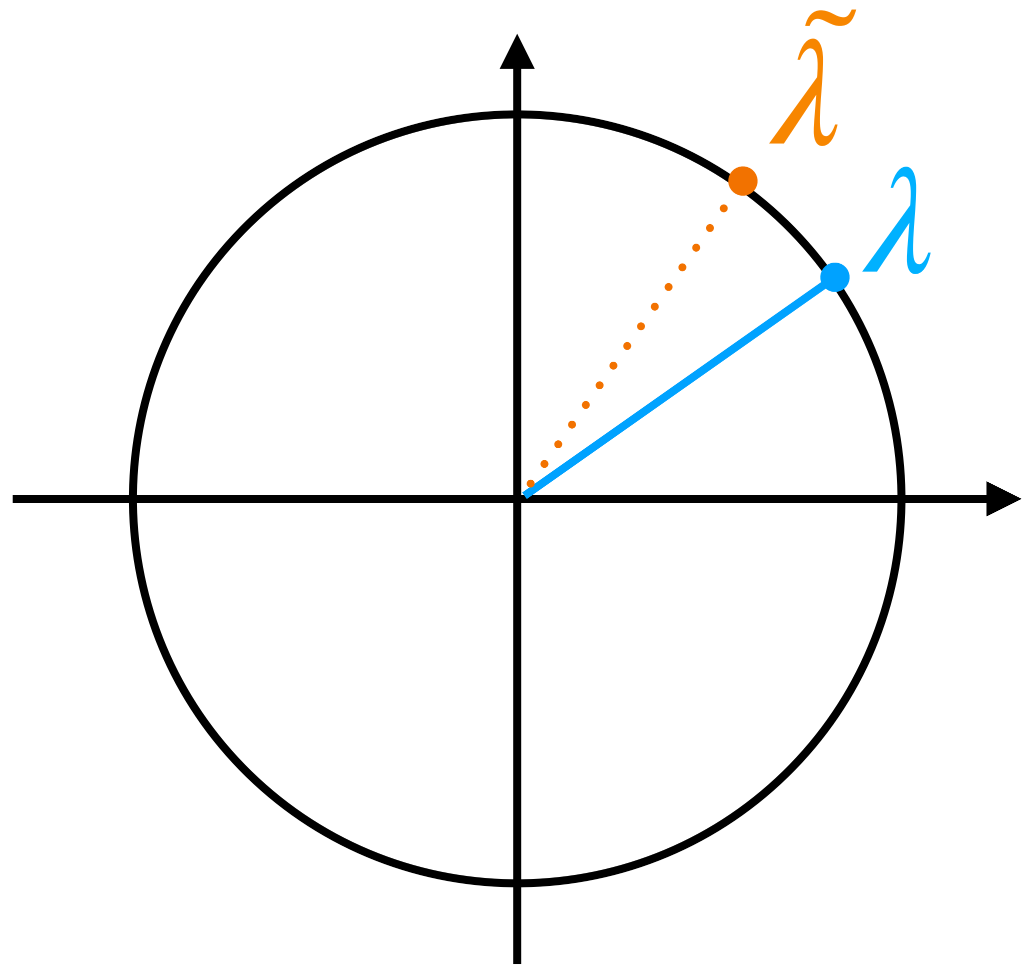


Quantum Phase Estimation

The textbook case

$$U|\phi\rangle = e^{2\pi i\theta}|\phi\rangle$$





$\tilde{\lambda} = e^{2\pi i\tilde{\theta}}$

$\lambda = e^{2\pi i\theta}$

$0 \leq \theta < 1$

✅ Optimal Heisenberg-limited scaling

⚡ Circuit depth scales inversely with error — even when $|\psi\rangle$ approaches eigenstate $|\phi\rangle$

$|\tilde{\theta} - \theta| \approx \epsilon$ using:

- $\mathcal{O}(1/\epsilon)$ c-U operations
- $\mathcal{O}(\log(1/\epsilon))$ ancillas

If $U = e^{iHt}$, then $\mathcal{O}(1/T)$ simulation time

[Kitaev 1995]

Hybrid Quantum Phase Estimation

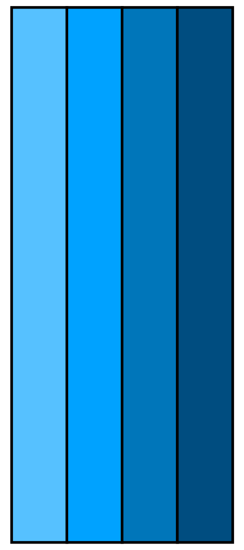
[Parish, McMahon 2019]

[Klymko, Mejuto-Zaera, Cotton et al 2022]

Subspace expansion through real-time evolution

$|\psi(t)\rangle = e^{-\mathrm{i}Ht}|\psi_0\rangle \longrightarrow$ Basis of n real-time expansion states

$$\left[\,|\psi(t_0)\rangle, |\psi(t_1)\rangle, |\psi(t_2)\rangle, \cdots, |\psi(t_{n-1})\rangle\right]$$



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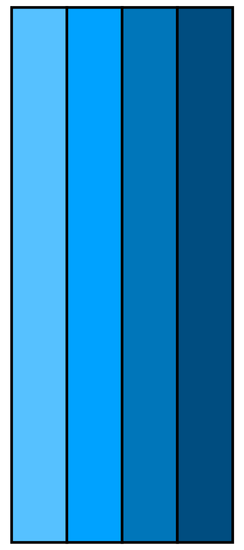
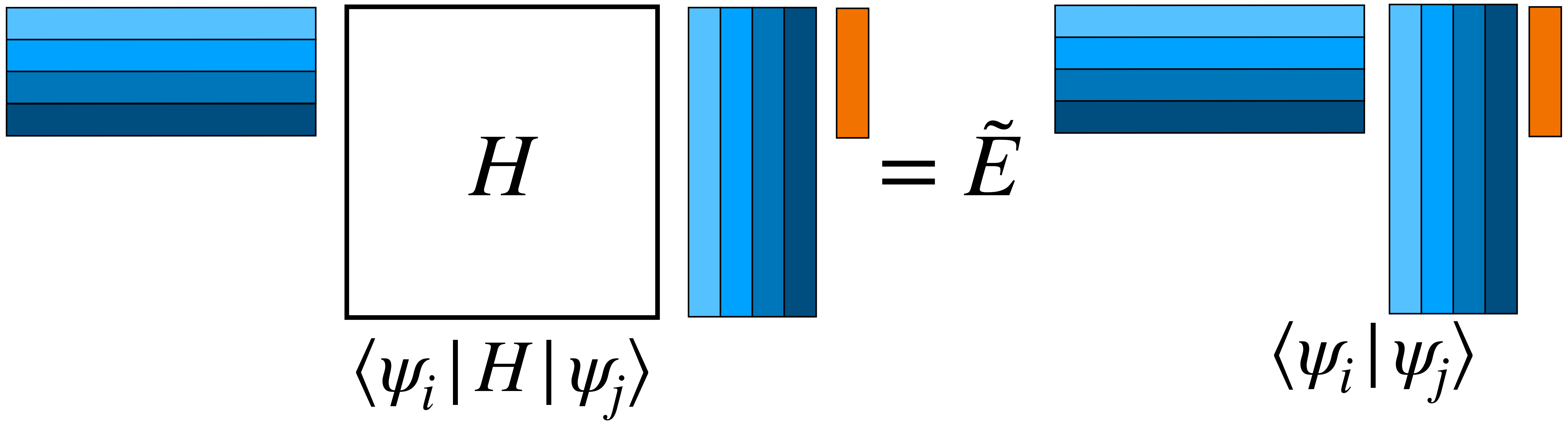


Rayleigh-Ritz procedure



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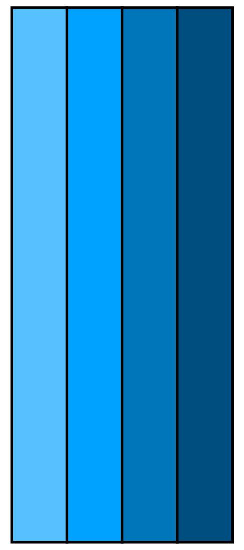
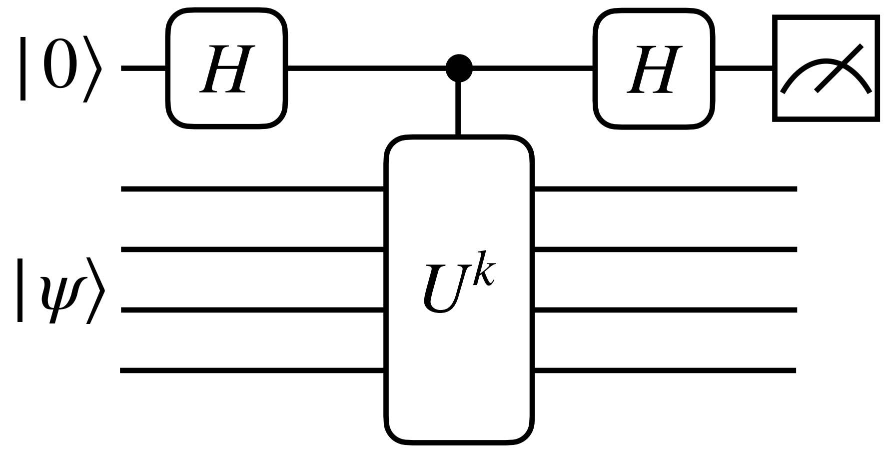
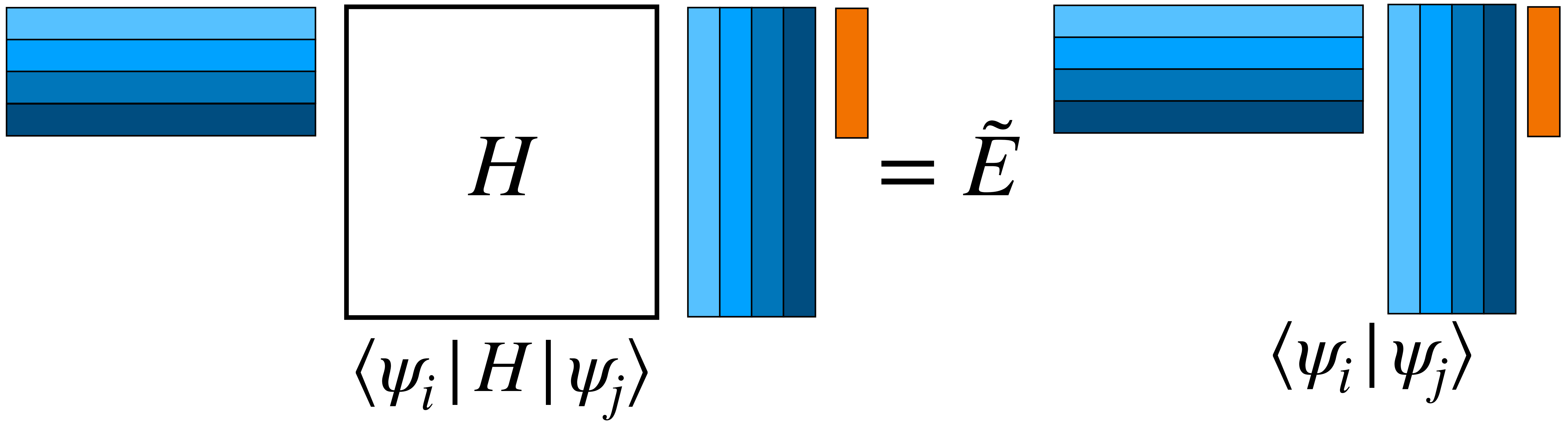


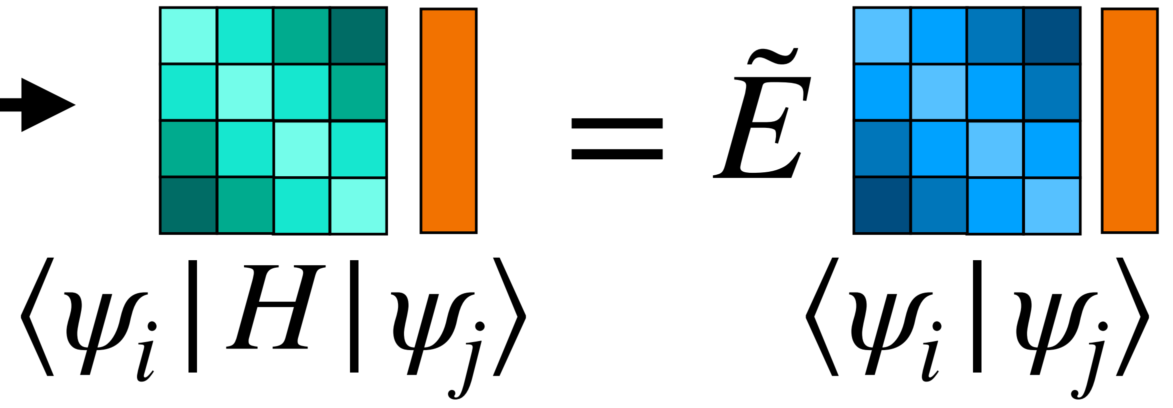


Hadamard test style circuit

Rayleigh-Ritz procedure



Small generalized eigenvalue problem (GEP)



Matrix elements measured on QC

Hybrid Quantum Phase Estimation

[Parish, McMahon 2019]

[Klymko, Mejuto-Zaera, Cotton et al 2022]

Subspace expansion through real-time evolution

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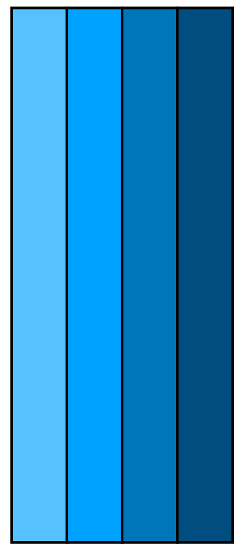

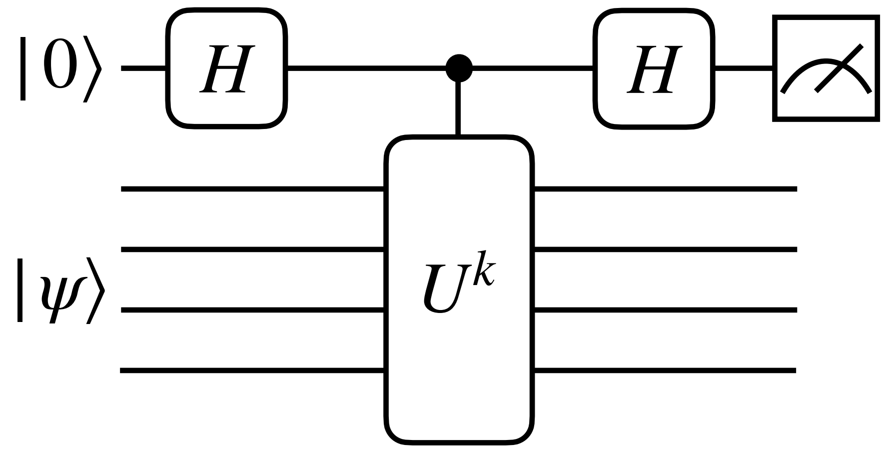

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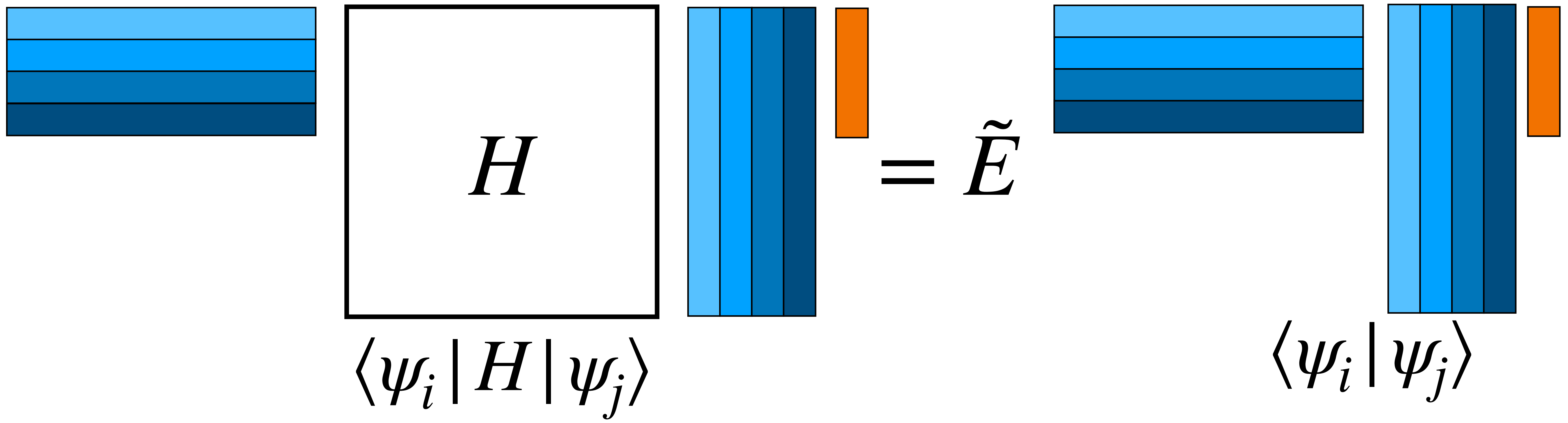

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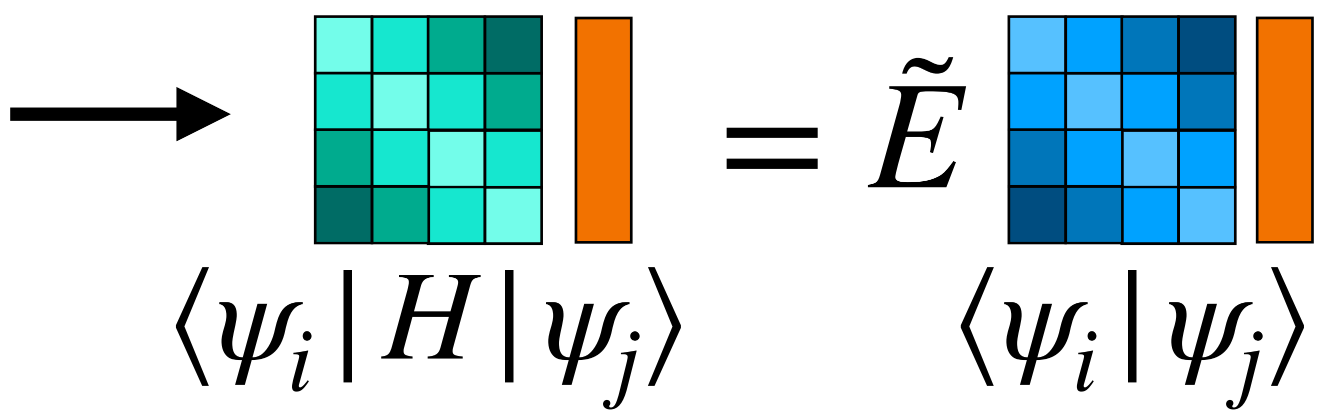


Matrix elements measured on QC

- ✅ Often converges to ground state manifold in few iterates with minimal conditions on $|\psi_0\rangle$
- ✅ Ritz vector provides low-dimensional representation of $|\psi_{\mathrm{GS}}\rangle$
- ⚡ GEP typically ill-conditioned, SVD regularization required [Epperly, Lin, Nakatsukasa 2022]
- ⚡ Trotterization destroys Toeplitz structure $\langle\psi_i|H|\psi_j\rangle \longrightarrow \mathcal{O}(n^2)$ matrix elements
- ⚡ $\mathcal{O}(1/\epsilon^2)$ Measurement cost

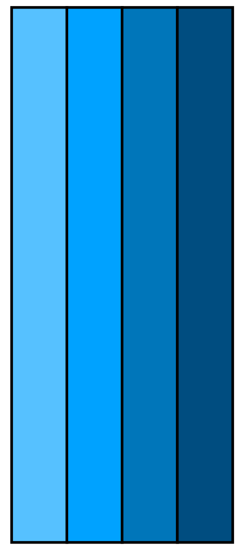
Hybrid Quantum Phase Estimation

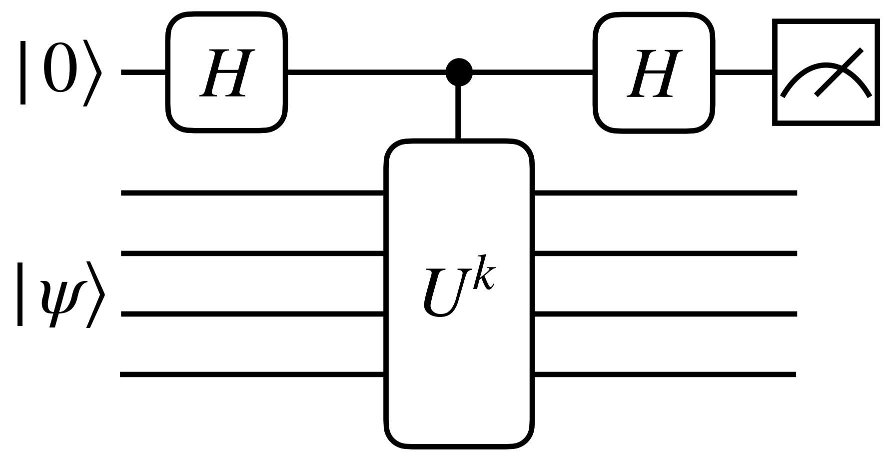
Subspace expansion through real-time evolution

[Klymko, Mejuto-Zaera, Cotton et al 2022]

$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle \longrightarrow$ Basis of n real-time expansion states

$$\left[|\psi(t_0)\rangle, |\psi(t_1)\rangle, |\psi(t_2)\rangle, \cdots, |\psi(t_{n-1})\rangle\right]$$





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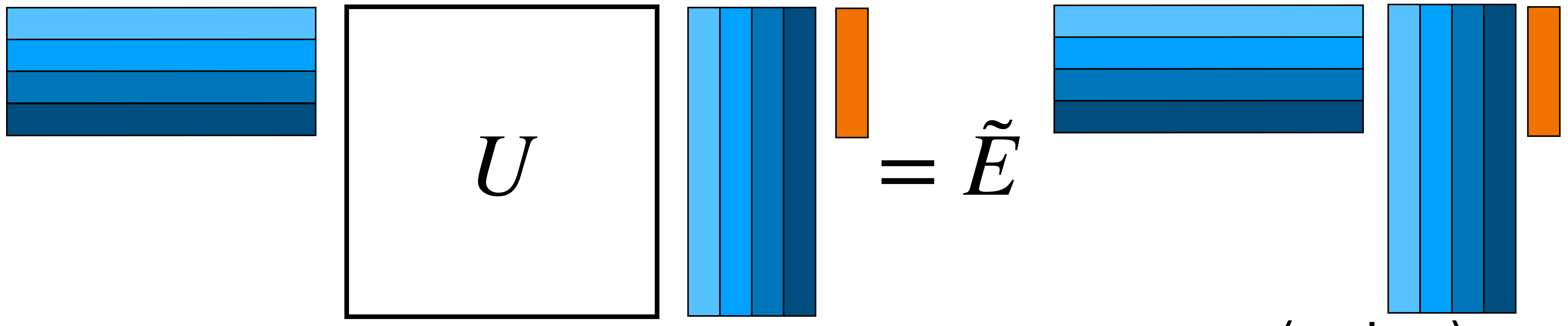
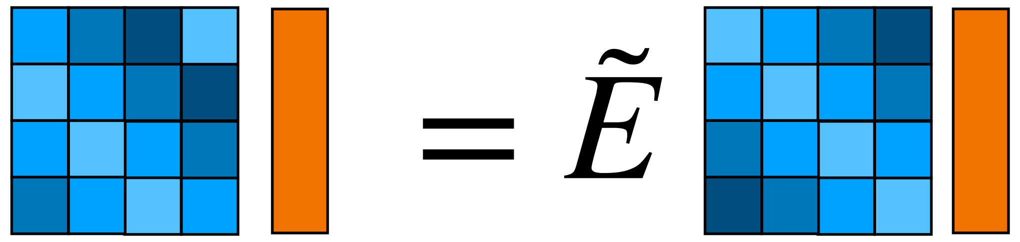


$\langle\psi_i|U|\psi_j\rangle$ $\langle\psi_i|\psi_j\rangle$

Small generalized eigenvalue problem (GEP)



$\langle\psi_i|U|\psi_j\rangle$ $\langle\psi_i|\psi_j\rangle$

Matrix elements measured on QC

$k \in \{0, \cdots, n-1\}$

$s_k = \langle\psi_0|U^k|\psi_0\rangle$

- ✅ Often converges to ground state manifold in few iterates with minimal conditions on $|\psi_0\rangle$
- ✅ Ritz vector provides low-dimensional representation of $|\phi_{GS}\rangle$
- ⚡ GEP typically ill-conditioned, SVD regularization required [Epperly, Lin, Nakatsukasa 2022]
- ⚡ ~~Trotterization destroys Toeplitz structure $\langle\psi_i|H|\psi_j\rangle \longrightarrow \mathcal{O}(n^2)$ matrix elements~~ ✅ $\mathcal{O}(n)$ matrix elements
- ⚡ $\mathcal{O}(1/\epsilon^2)$ Measurement cost

Hybrid Quantum Phase Estimation

A Signal Processing Point of View

$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle = \sum_n \langle\phi_n|\psi_0\rangle\, e^{-iE_n t}|\phi_n\rangle \longrightarrow s_k = \langle\psi_0|U^k|\psi_0\rangle = \sum_n |c_n|^2 \lambda_n^k$$

$\langle\phi_n|\psi_0\rangle \to c_n$, $e^{-iE_n t} \to \lambda_n^t$

$$H = \sum_n E_n |\phi_n\rangle\langle\phi_n|$$

Sum-of-sinusoids

Hybrid Quantum Phase Estimation

A Signal Processing Point of View

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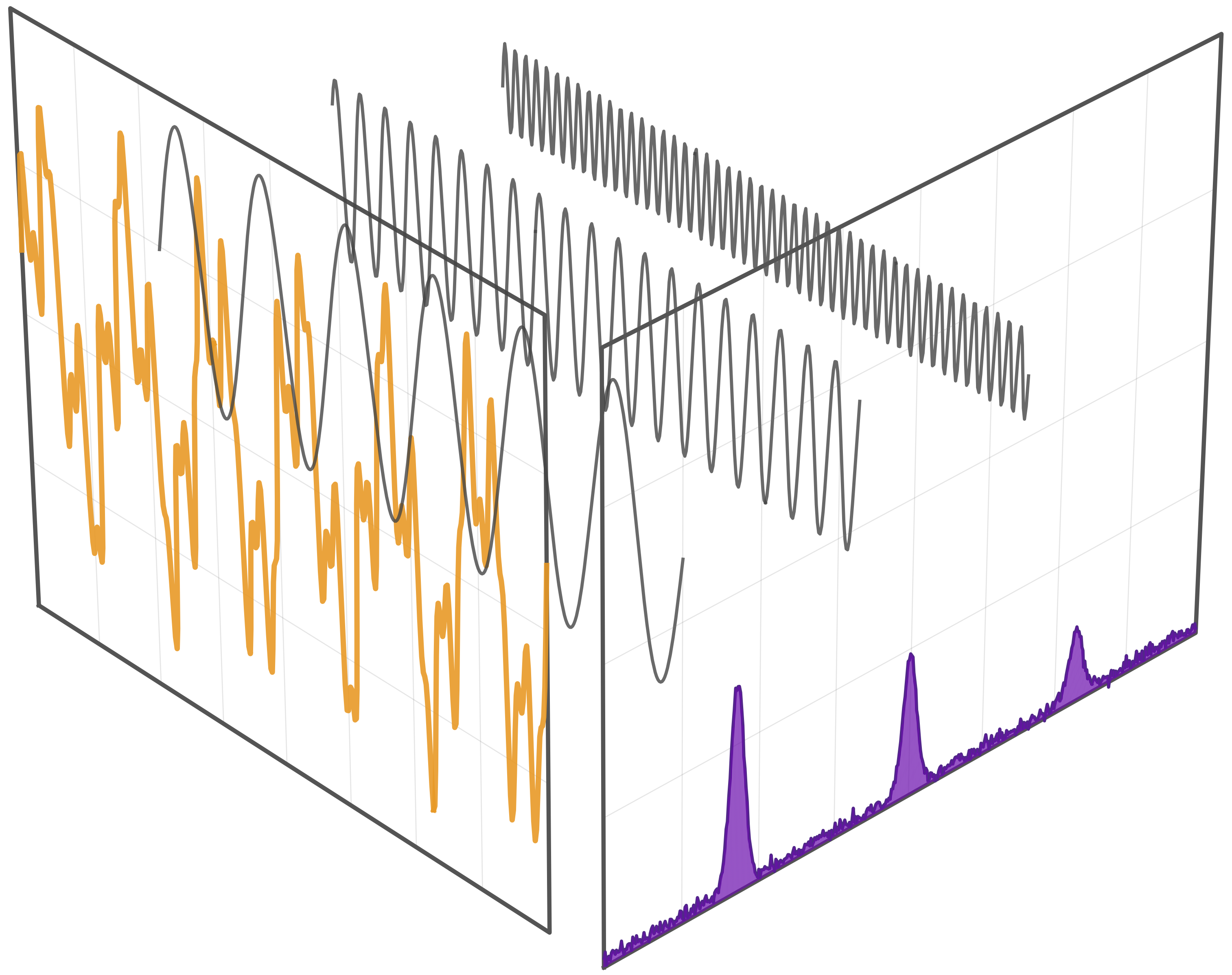
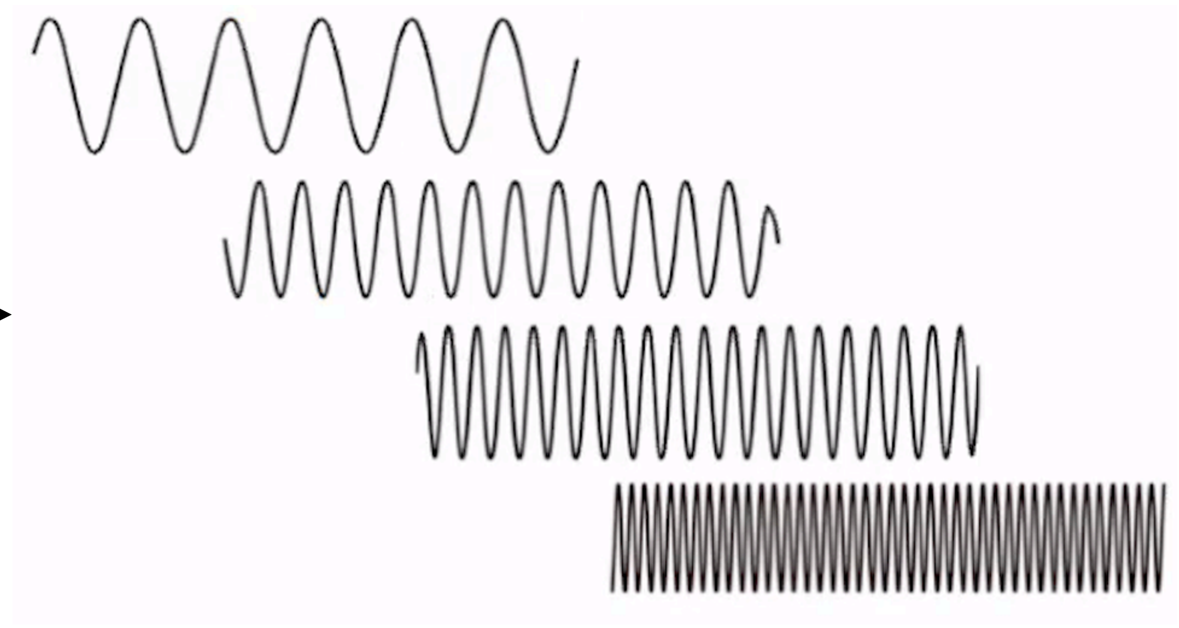
Sum-of-sinusoids





Filtering methods to isolate out dominant modes

Hybrid Quantum Phase Estimation

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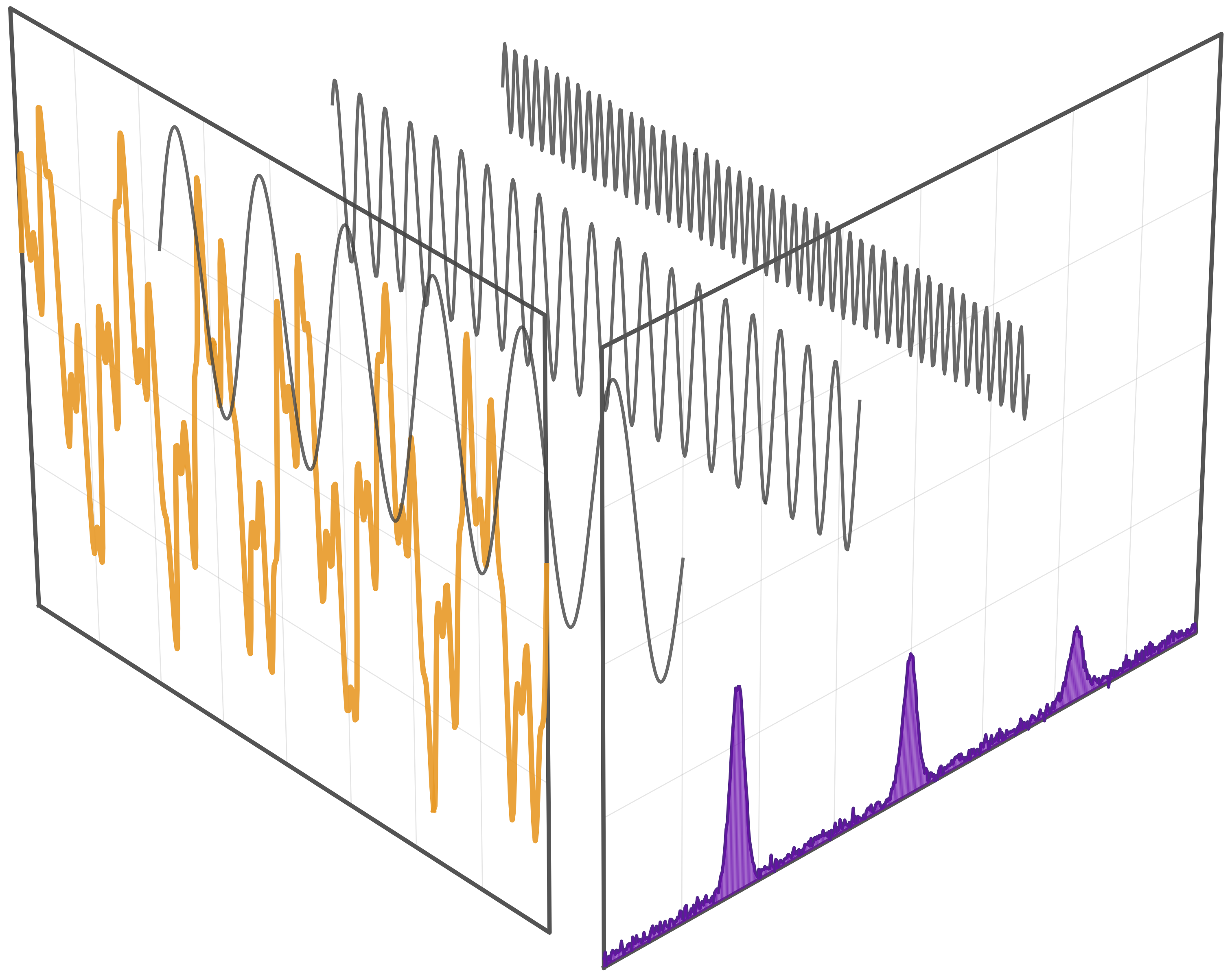
Sum-of-sinusoids



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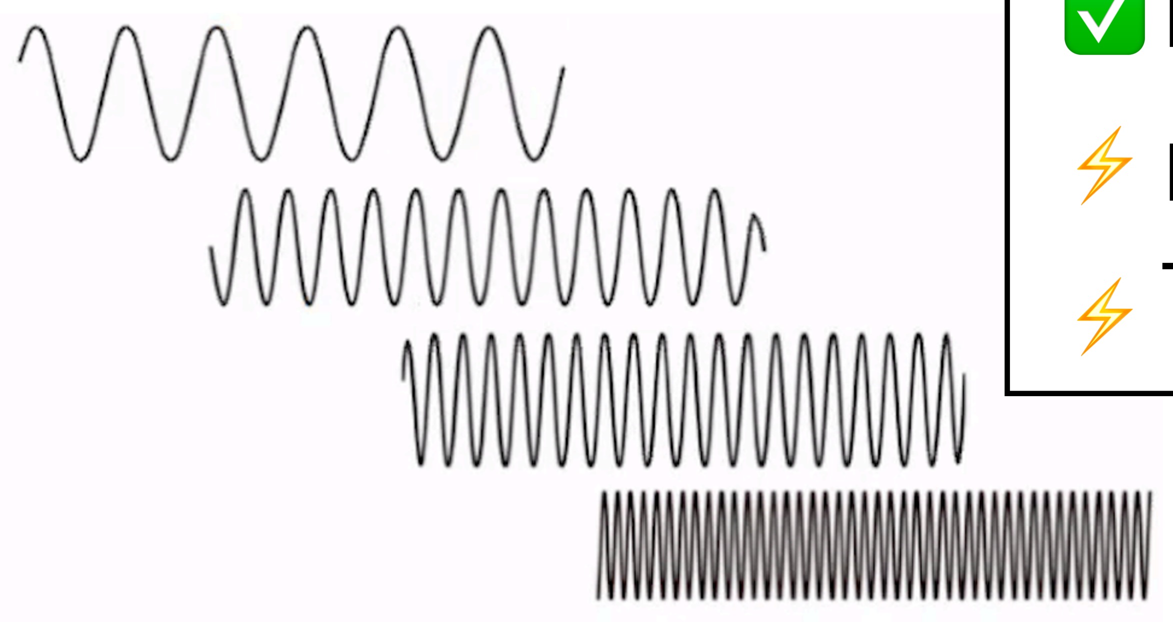


Filtering methods to isolate out dominant modes

- ✅ Robust convergence to eigenvalues
- ✅ No ill-conditioned GEP
- ⚡ No representation of $|\phi_{GS}\rangle$
- ⚡ Typically stricter conditions on $|\psi_0\rangle$

[Ding, Lin 2023]

[Shen, Camps, Szasz et al 2025]

Observable Dynamic Mode Decomposition (ODMD)

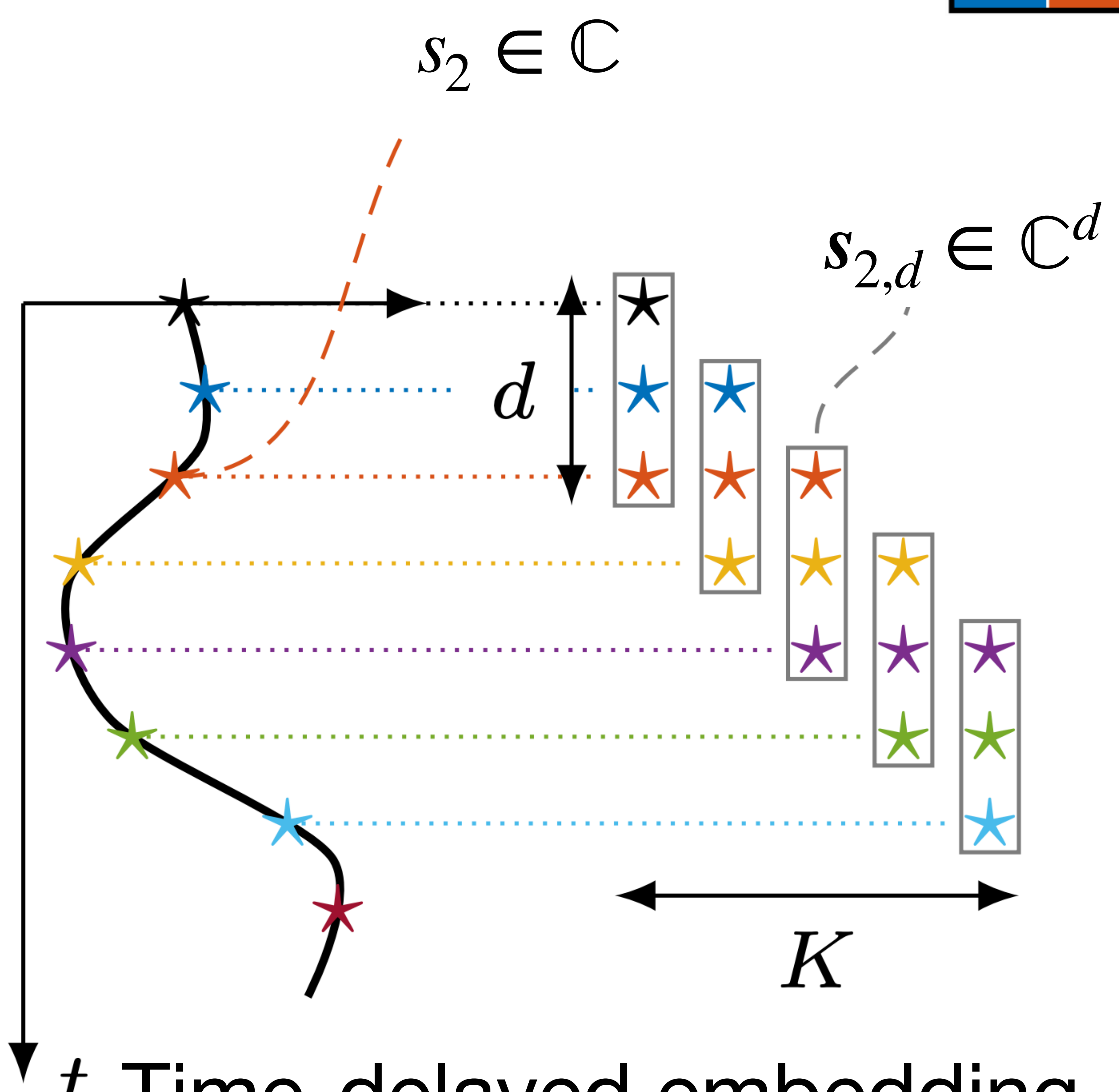
Observable Dynamic Mode Decomposition

$$s_k = \sum_n |c_n|^2 \lambda_n^k$$

Sum-of-sinusoids

Time series of "observables"

$$[s_0, s_1, s_2, s_3, s_4, s_5, s_6]$$



Time-delayed embedding

Dynamic Mode Decomposition: model reduction for complex fluid processes

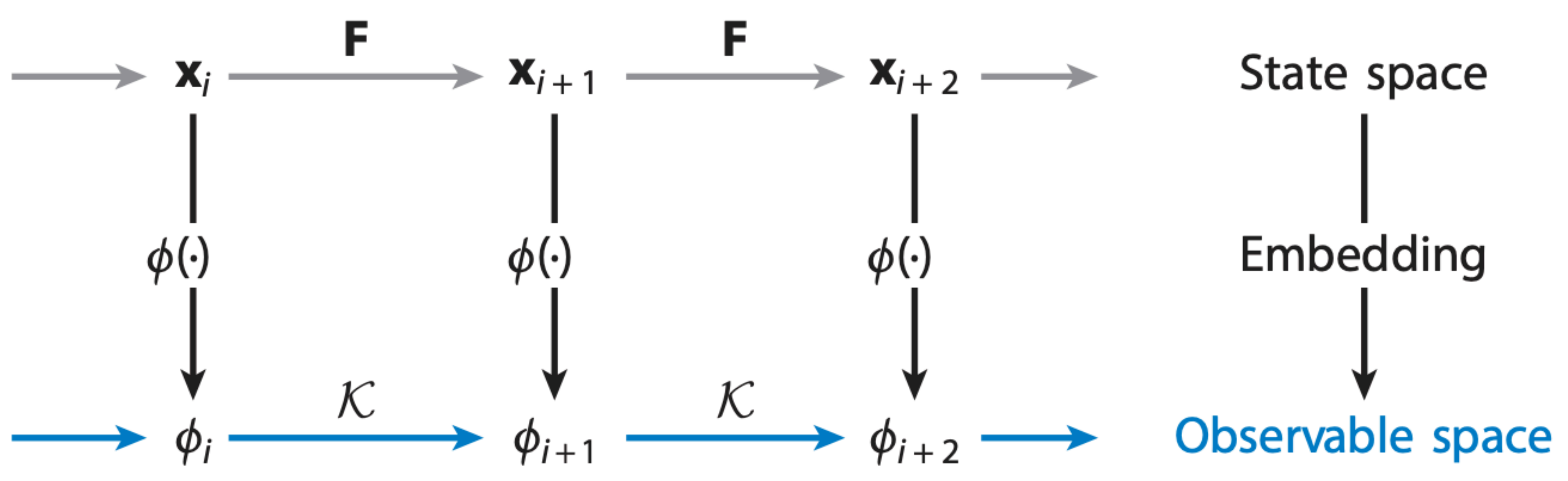


Figure 1

Projection of the state space dynamics given by a nonlinear mapping **F** onto the dynamics in an infinite-dimensional observable space given by the linear Koopman operator $\mathcal{K}$. We use the notation $\phi_i = \phi(\mathbf{x}_i)$, where $\mathbf{x}_i$ are state variables for the i-th snapshot and ϕ_i are the observables for the i-th snapshot.

[Shmid 2022]

[Shen, Camps, Szasz et al 2025]

Observable Dynamic Mode Decomposition

$$s_k = \sum_n |c_n|^2 \lambda_n^k$$

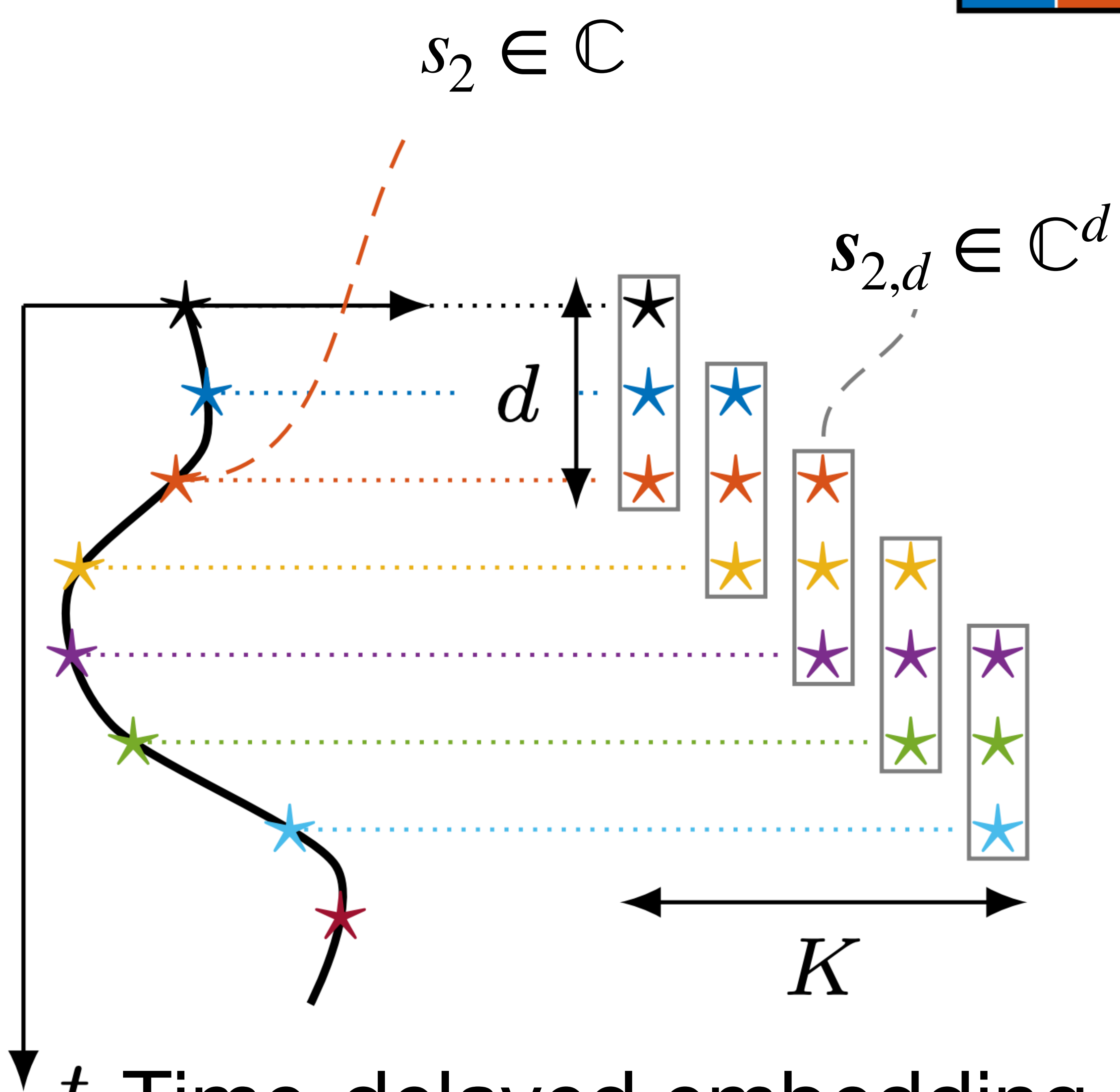
Sum-of-sinusoids

Time series of “observables”

$$[s_0, s_1, s_2, s_3, s_4, s_5, s_6]$$

Snapshots of “observables”

$$[\mathbf{s}_{0,d}, \mathbf{s}_{1,d}, \mathbf{s}_{2,d}, \mathbf{s}_{3,d}, \mathbf{s}_{4,d}]$$



Time-delayed embedding

[Shen, Camps, Szasz et al 2025]

Observable Dynamic Mode Decomposition

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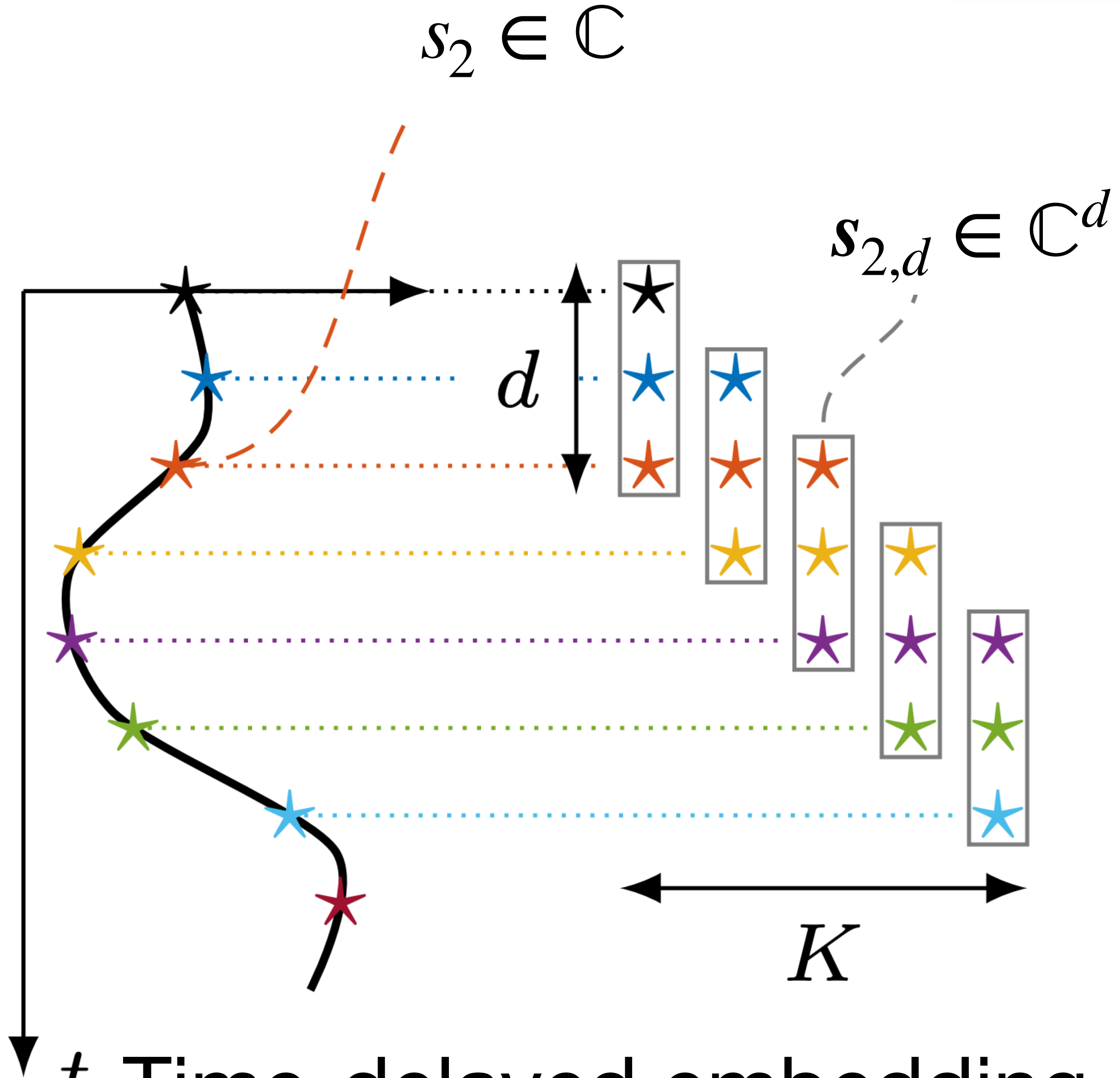


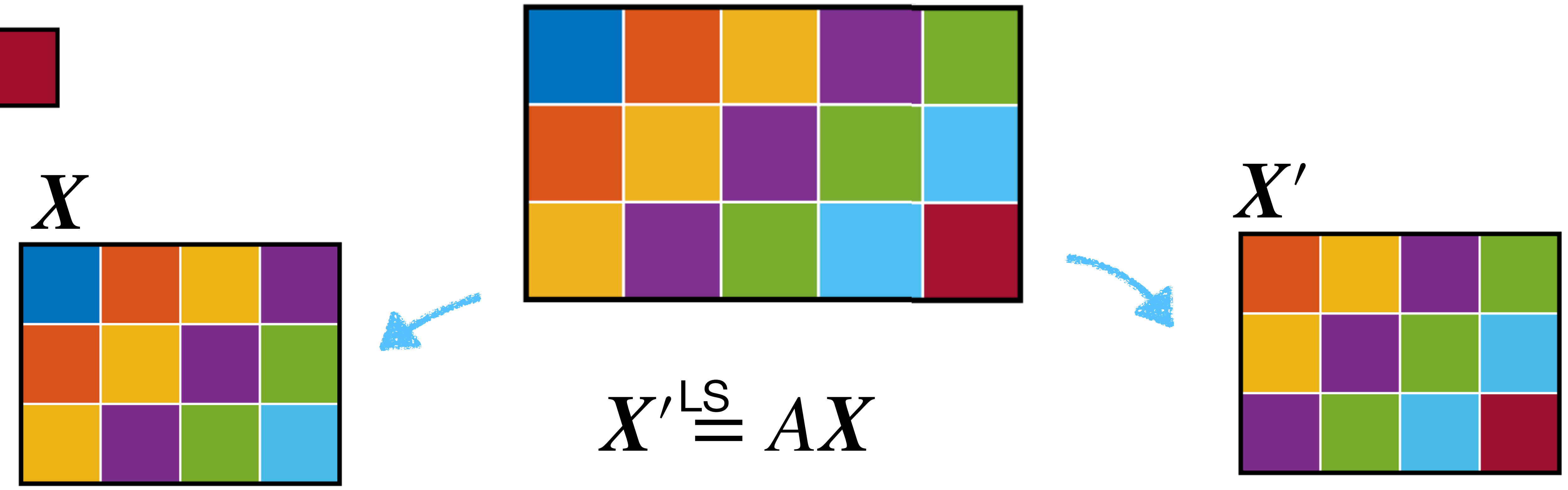
Time-delayed embedding

Time series of "observables"

$[s_0, s_1, s_2, s_3, s_4, s_5, s_6]$

Snapshots of "observables"

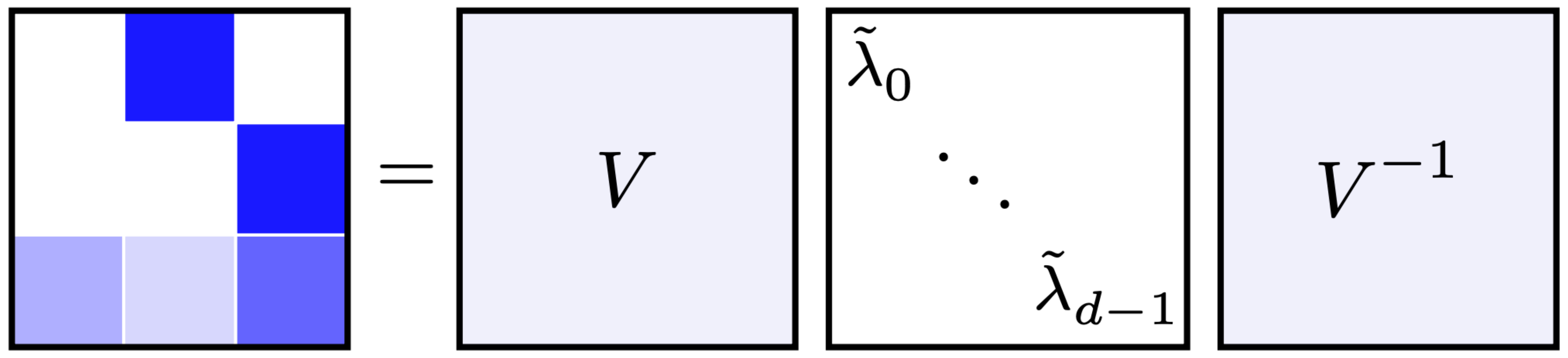
$[\boldsymbol{s}_{0,d}, \boldsymbol{s}_{1,d}, \boldsymbol{s}_{2,d}, \boldsymbol{s}_{3,d}, \boldsymbol{s}_{4,d}]$



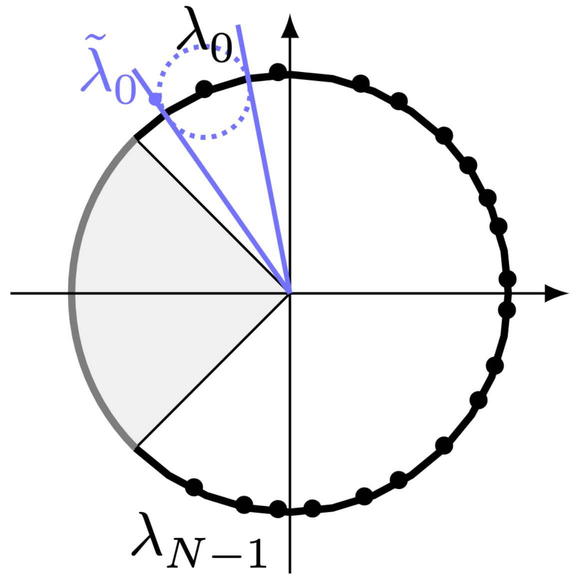
$$\boldsymbol{X}' \overset{\text{LS}}{=} A\boldsymbol{X}$$

System matrix: $A = \boldsymbol{X}'\boldsymbol{X}^+ \approx U$

$A \in \mathbb{R}^{d \times d}$



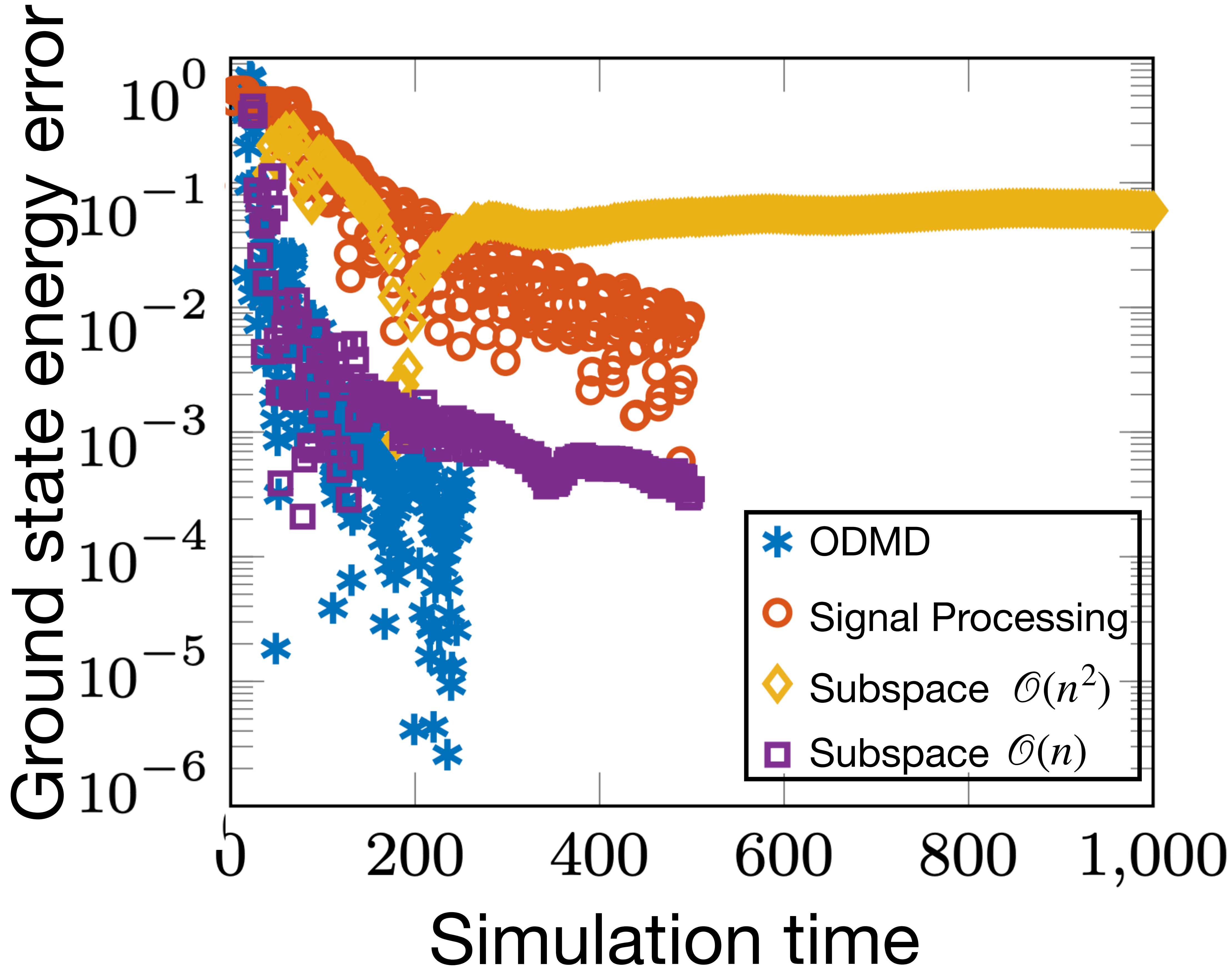
Companion structure



$-\arg \tilde{\lambda}_0 \approx E_0$

[Shen, Camps, Szasz et al 2025]

Robust convergence to ground state energy



1D Heisenberg model on 12 sites

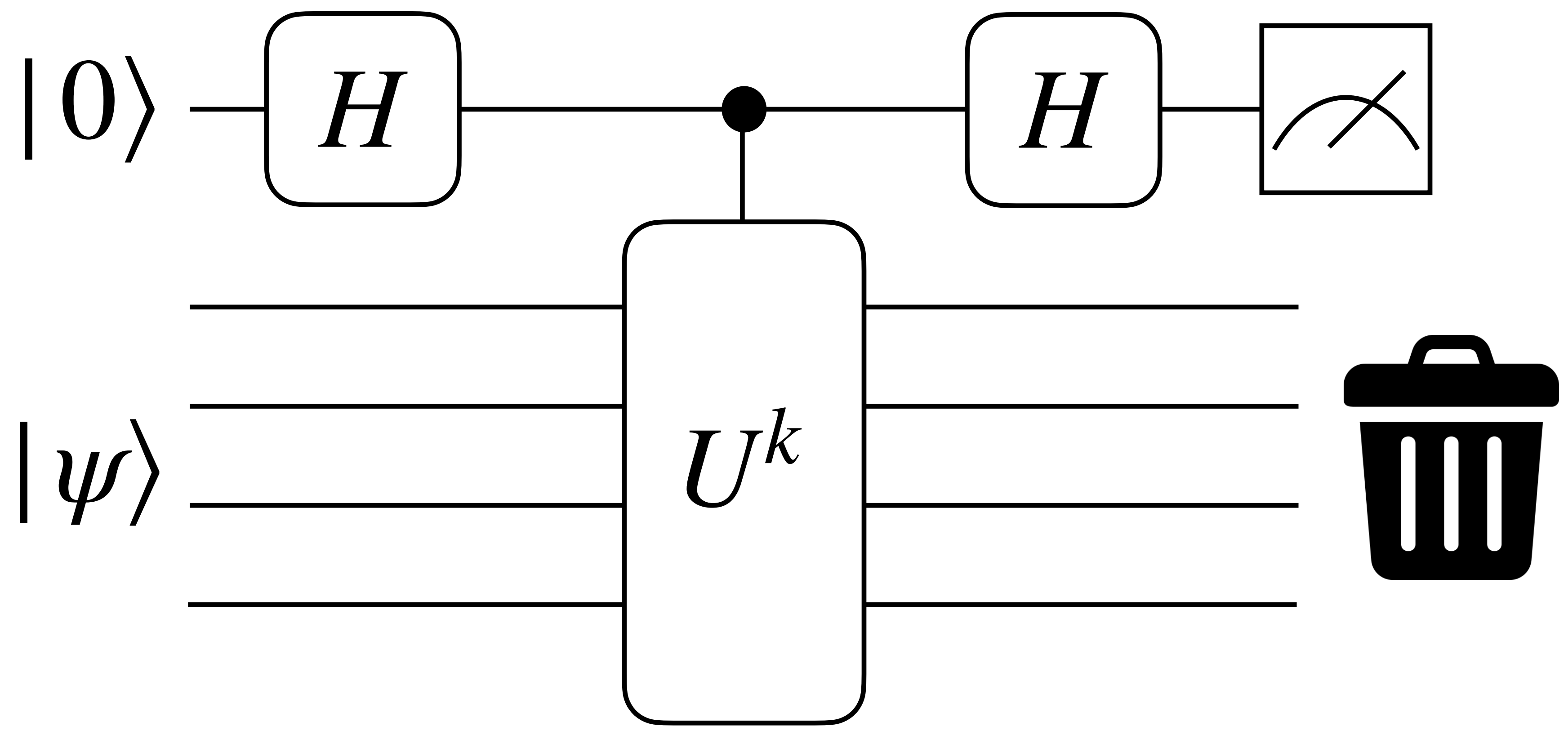
$$H = J \sum \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}$$

ODMD is:

- A **signal processing method** ≅ matrix pencil methods (ESPRIT)
- A **subspace method**
  - Two-sided Krylov method on Hilbert space
  - Function Krylov method of Koopman operator

Can we collect more data from the same number of circuit runs?

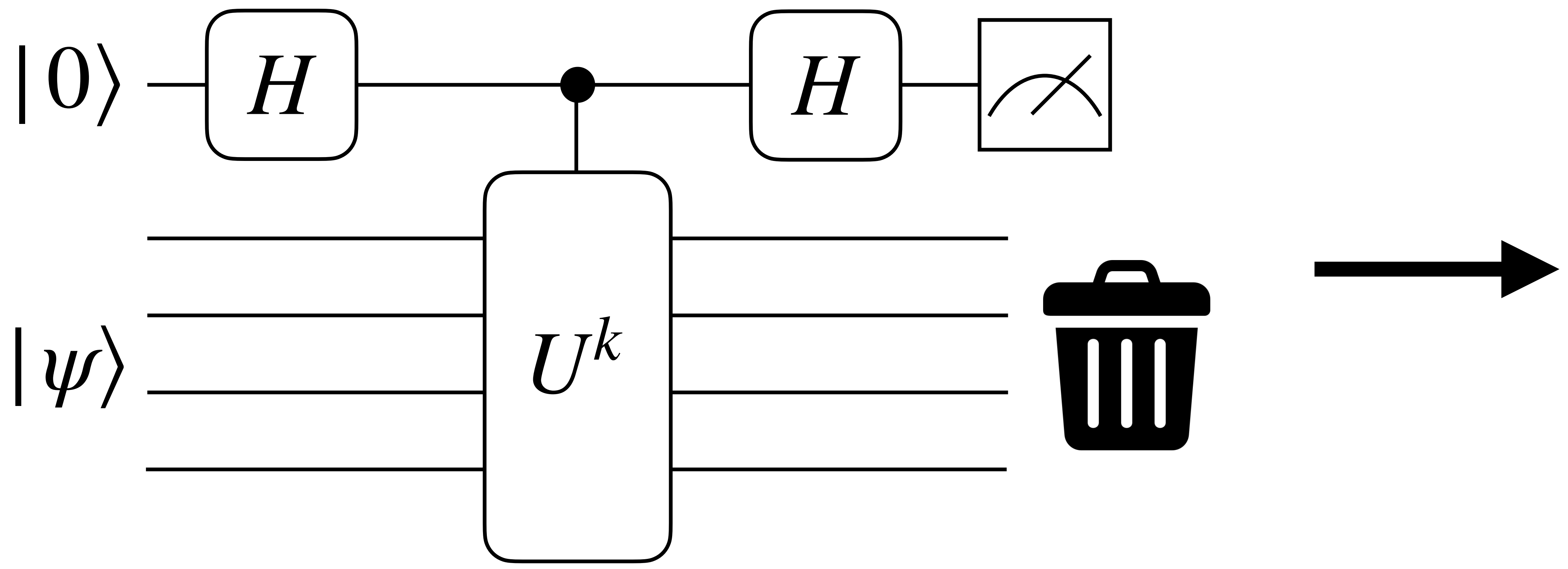
Hadamard test circuit



$$s_k = \langle \psi_0 | U^k | \psi_0 \rangle$$

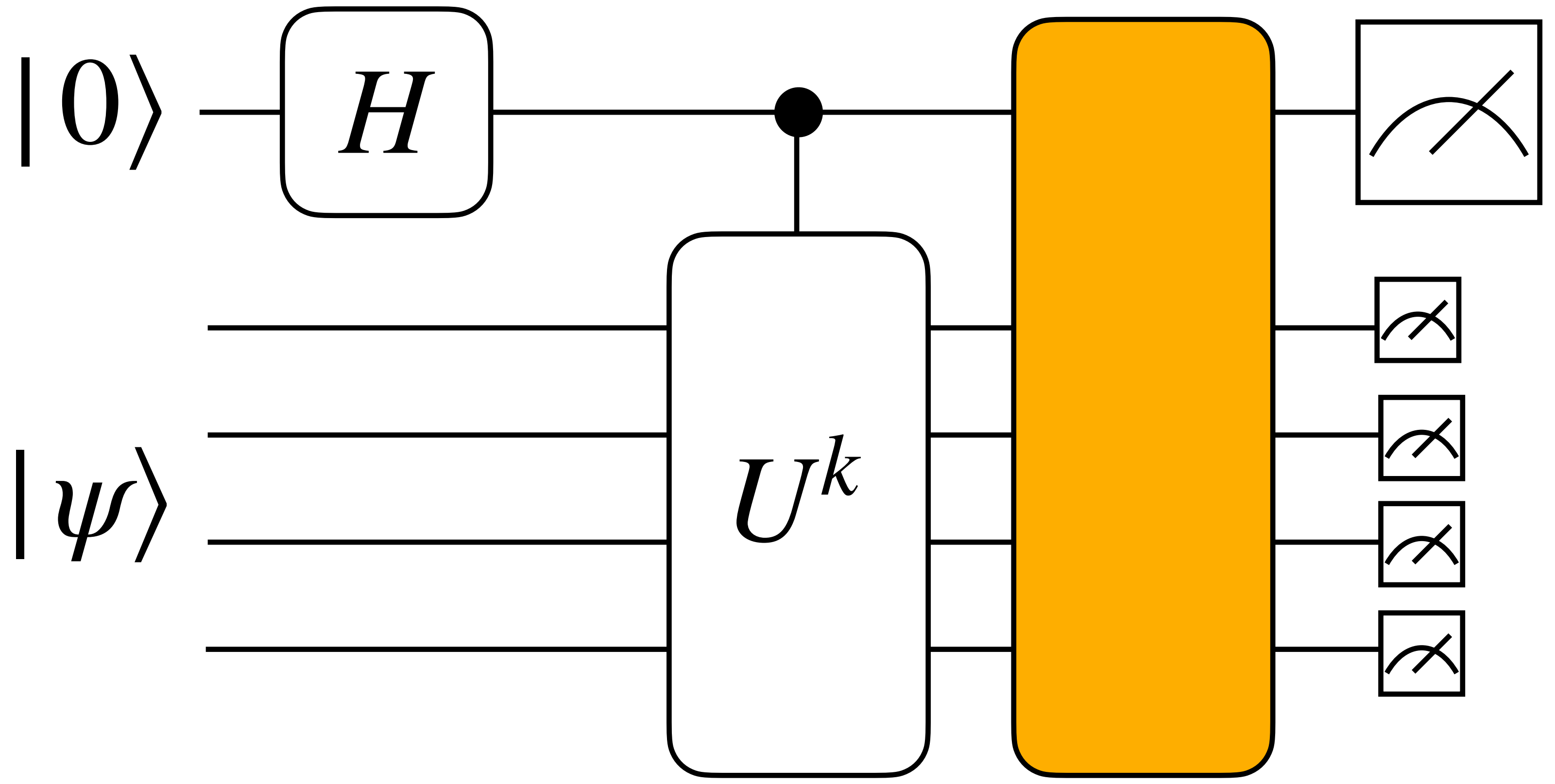
Can we collect more data from the same number of circuit runs?

Hadamard test circuit



$$s_k = \langle \psi_0 | U^k | \psi_0 \rangle$$

Measure all the qubits



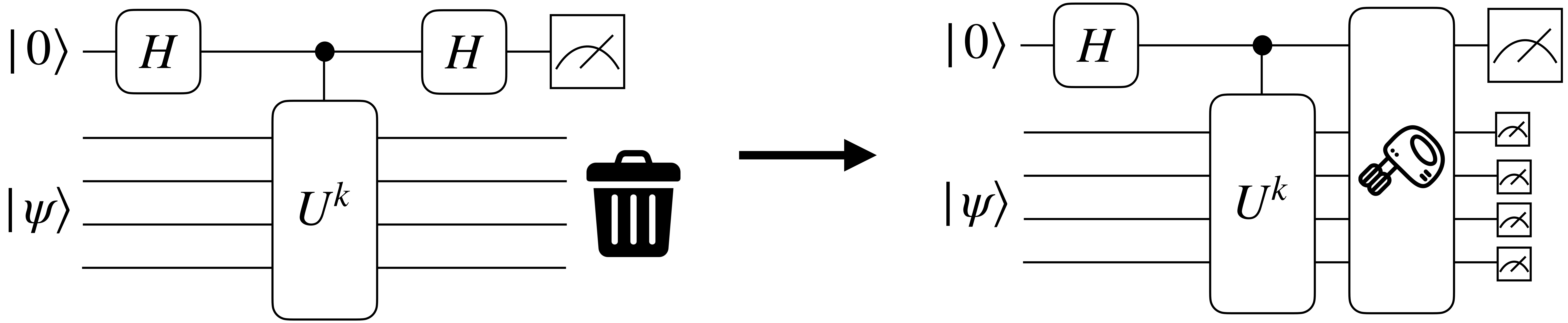
What if we measure all qubits and squeeze out more information?

$$\mathbf{s}_k = \left[\langle \psi_0 | O_1 U^k | \psi_0 \rangle, \langle \psi_0 | O_2 U^k | \psi_0 \rangle, \cdots, \langle \psi_0 | O_L U^k | \psi_0 \rangle \right]$$

Can we collect more data from the same number of circuit runs?

Hadamard test circuit

Measure all the qubits



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$$\boldsymbol{s}_k = \left[\langle \psi_0 | O_1 U^k | \psi_0 \rangle, \langle \psi_0 | O_2 U^k | \psi_0 \rangle, \cdots, \langle \psi_0 | O_L U^k | \psi_0 \rangle \right]$$

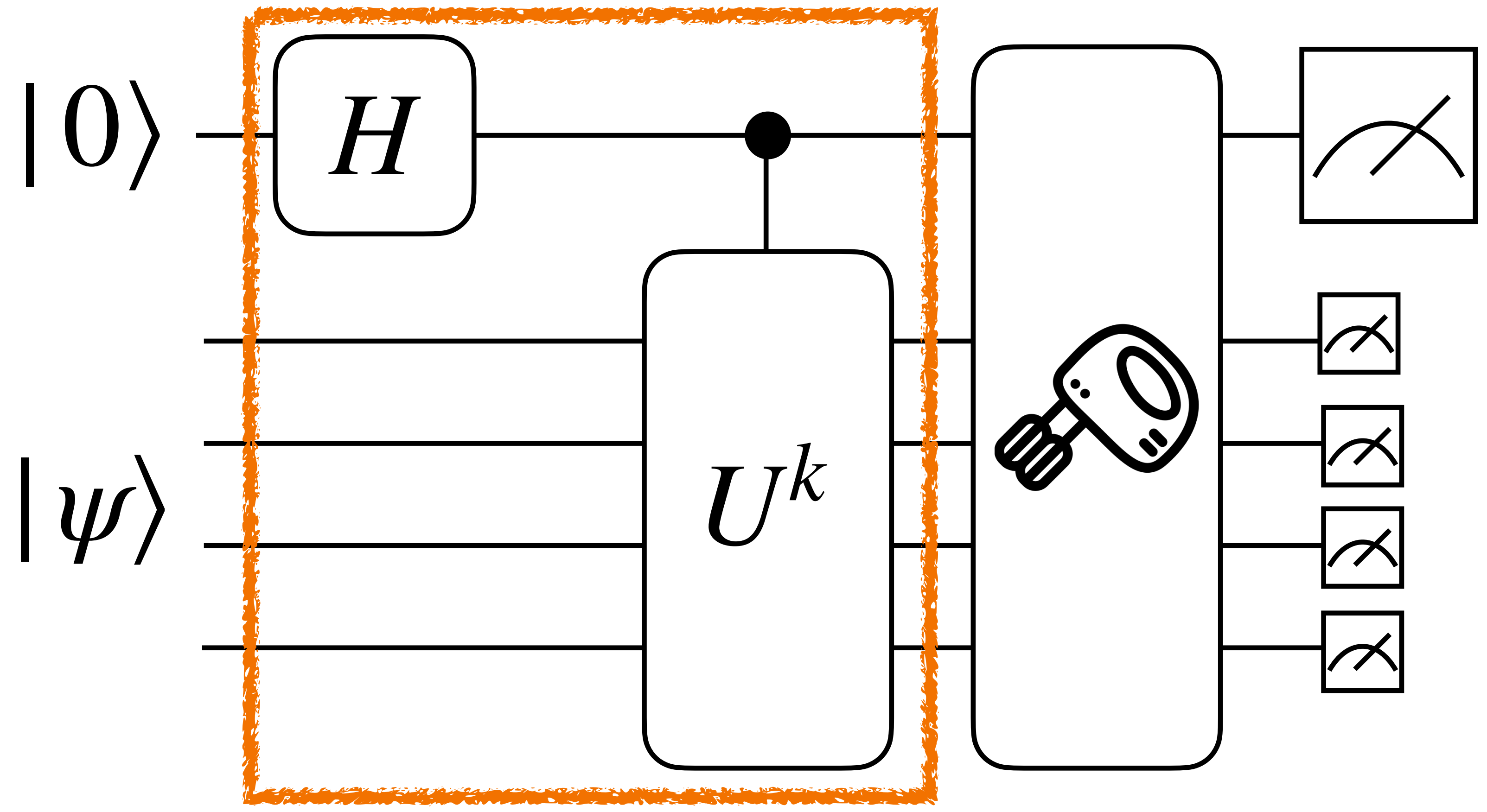
💡 Multi-Observable Dynamic Mode Decomposition (**MODMD**)

[Shen, Buzali, Hu et al 2026]

Scrambling unitary of depth $\log(n)$ ✅

The Quantum Side of MODMD

Shallow Shadows



$\rho(t_k) = |\Psi(t_k)\rangle\langle\Psi(t_k)|$

Shadow dataset

010…010
111…001
100…101
…

[Huang, Kueng, Preskill 2020]

Predict (many) properties of ρ

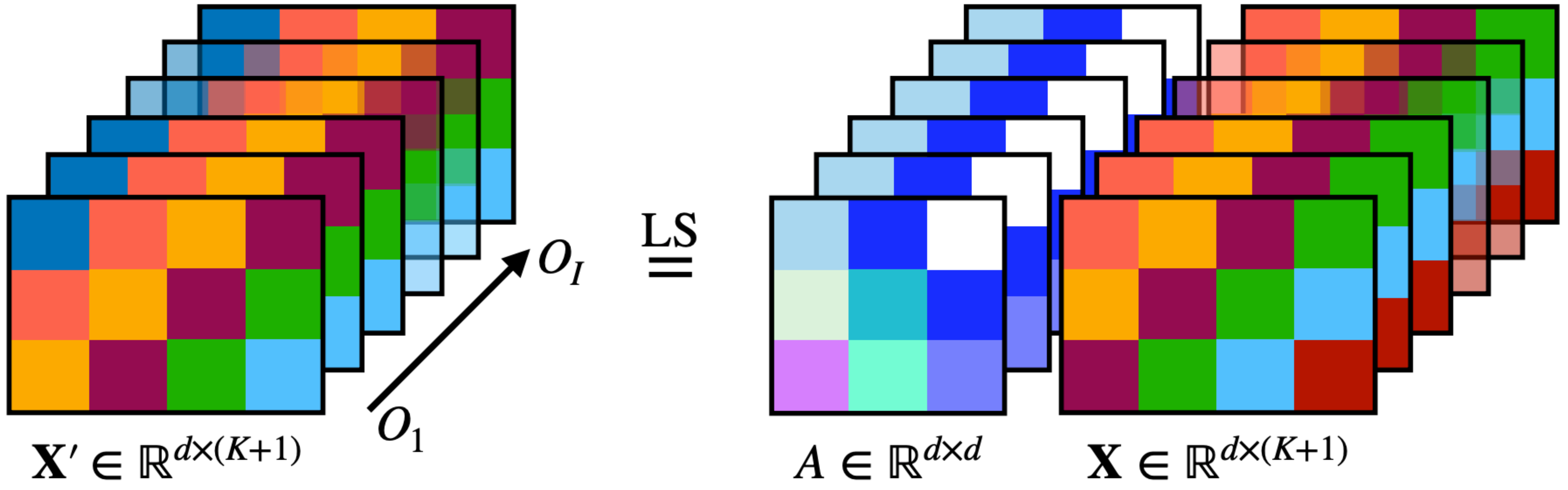
$\langle\psi_0|O_i U^k|\psi_0\rangle$

- O_i? 1-qubit, 2-qubit, …, n-qubit
- $s_k = \left[\langle\psi_0|O_1 U^k|\psi_0\rangle, \langle\psi_0|O_2 U^k|\psi_0\rangle, \cdots, \langle\psi_0|O_L U^k|\psi_0\rangle\right]$
- Variance $\propto \dfrac{\log(L)\max_i \|O_i^2\|}{N}$

The Classical Side of MODMD

Input: multi-observable signal from constructed from shadows

$$\boldsymbol{s}_k = \left[\langle\psi_0|O_1U^k|\psi_0\rangle, \langle\psi_0|O_2U^k|\psi_0\rangle, \cdots, \langle\psi_0|O_IU^k|\psi_0\rangle\right]$$

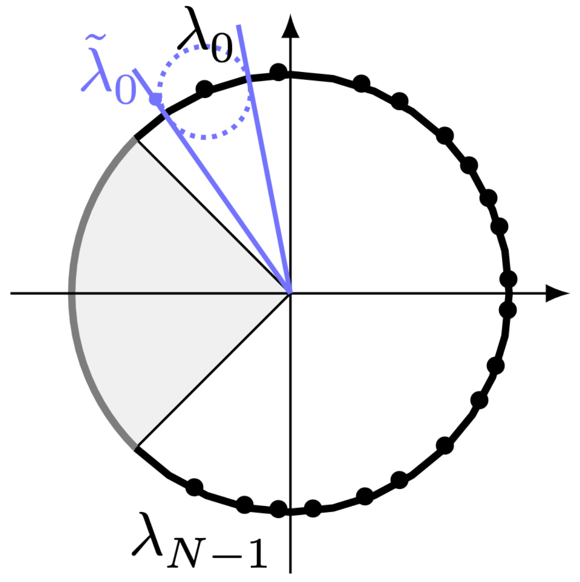


$$\underbrace{\begin{bmatrix} \vec{s}_1 & \vec{s}_2 & \cdots & \vec{s}_{K+1} \\ \vec{s}_2 & \vec{s}_3 & \cdots & \vec{s}_{K+2} \\ \vdots & \vdots & \ddots & \vdots \\ \vec{s}_d & \vec{s}_{d+1} & \cdots & \vec{s}_{K+d} \end{bmatrix}}_{\mathbf{X}'\in\mathbb{R}^{dI\times(K+1)}} \overset{\text{LS}}{=} A \underbrace{\begin{bmatrix} \vec{s}_0 & \vec{s}_1 & \cdots & \vec{s}_K \\ \vec{s}_1 & \vec{s}_2 & \cdots & \vec{s}_{K+1} \\ \vdots & \vdots & \ddots & \vdots \\ \vec{s}_{d-1} & \vec{s}_d & \cdots & \vec{s}_{K+d-1} \end{bmatrix}}_{\mathbf{X}\in\mathbb{R}^{dI\times(K+1)}}$$

✅ Block Krylov subspace method

✅ If $|c_0|^2 > 1/2$ then circuit depth $\mathcal{O}((1/|c_0|^2 - 1)/\epsilon)$
If $|c_0|^2 > 8/9$ then circuit depth $\tilde{\mathcal{O}}((1/\epsilon^{2/3})$
With shot noise $\epsilon_{\text{noise}} = \mathcal{O}(1)$ [Ding, Epperly, Lin, Zhang, 2024]

Diagonalize A →

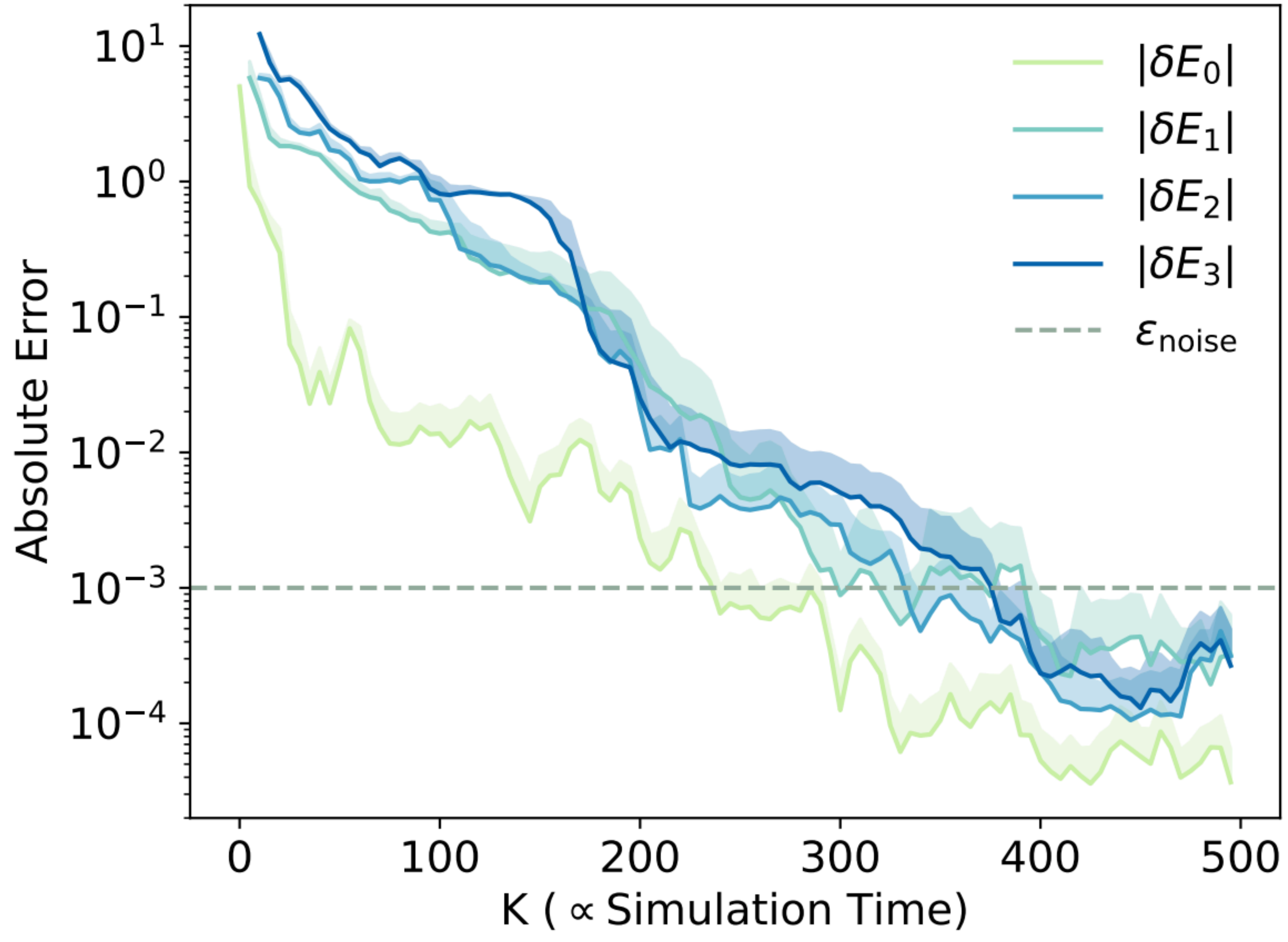


$-\arg\tilde{\lambda}_0 \approx E_0$

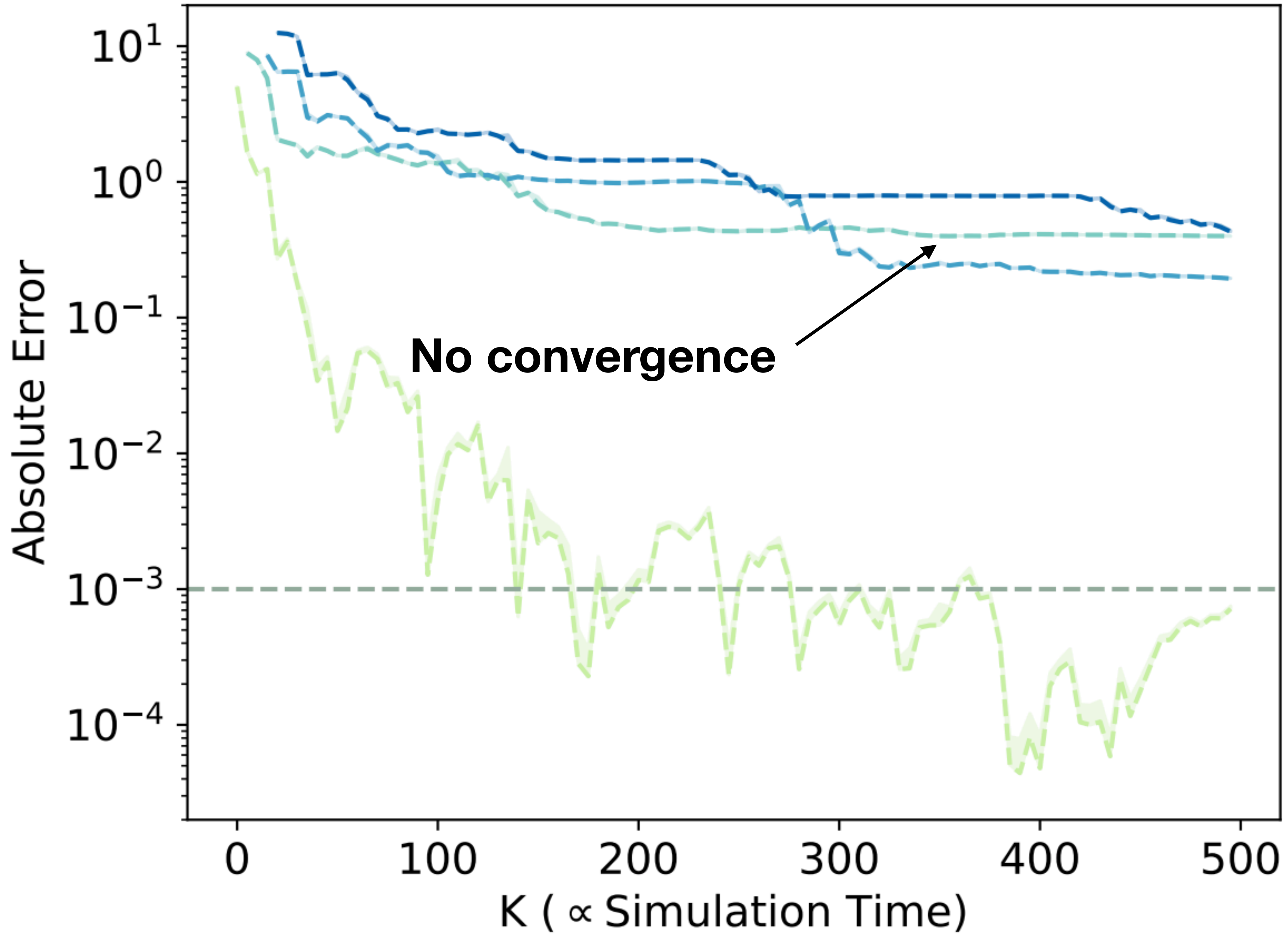
Robust convergence to low-lying energies

1D Spin chain with 15 sites

MODMD (7 observables)



ODMD (1 observable)

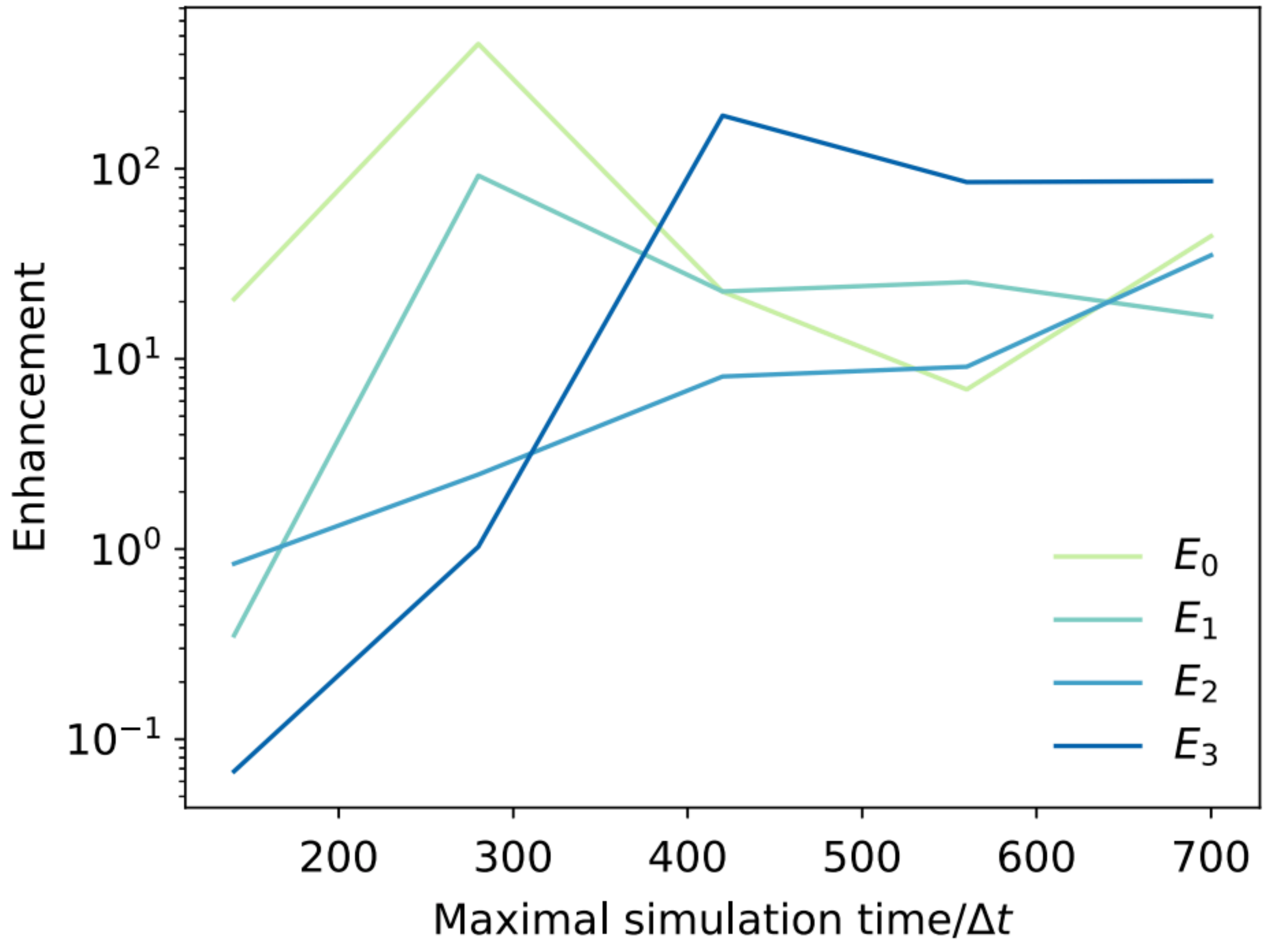


Robust convergence to low-lying energies

1D Spin chain with 15 sites

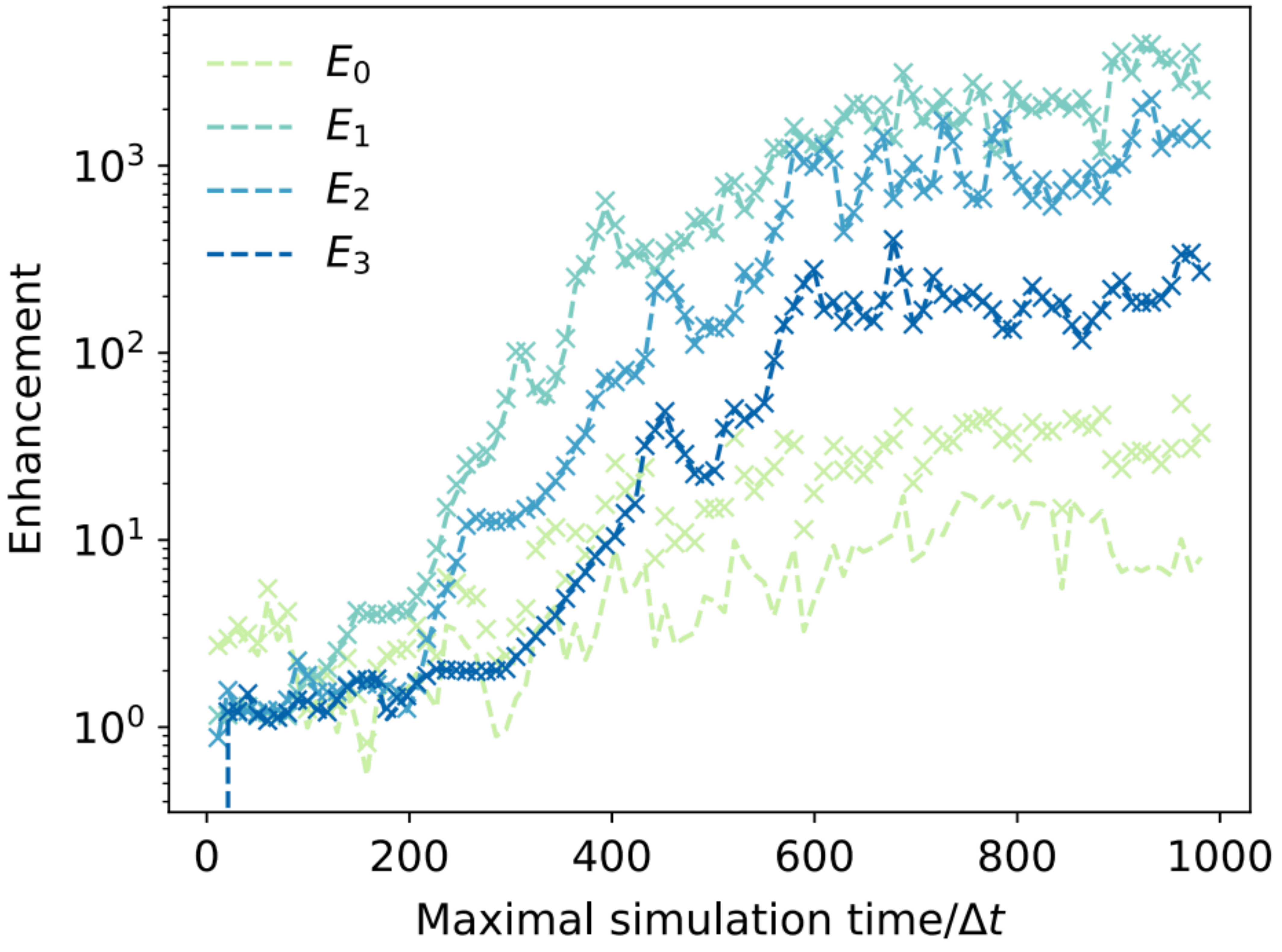
7 observables

MODMD v QMEGS



[Ding, Li, Lin et al 2022]

MODMD v (U)VQPE



[Klymko, Mejuto-Zaera, Cotton et al 2022]

Part II. Evaluating matrix functions.

Computing functions of operators

An algorithmic primitive with many applications

$\langle \psi_0 | f(U) | \psi_0 \rangle$

Given query access to U $\longrightarrow$ Compute properties of $f(U)$

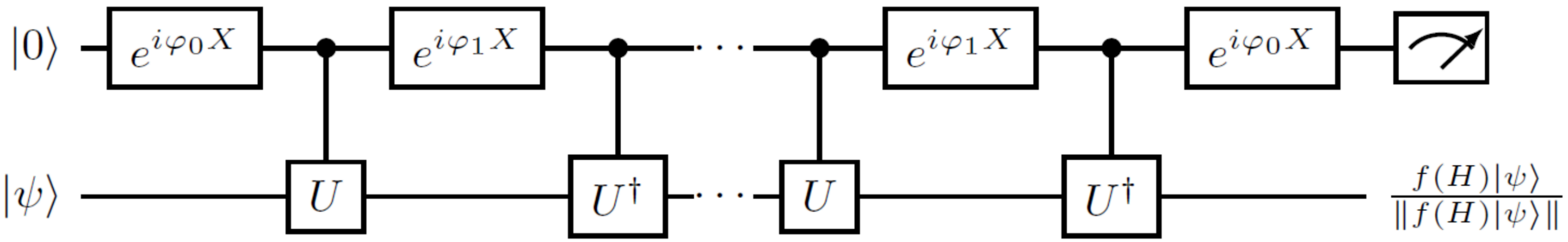
Gibbs sampling
$\rho = e^{-\beta H}/Z$

Linear systems
H^{-1}

Green's functions
$G(\omega) = (H - \omega - i\chi)^{-1}$

Quantum Eigenvalue Transformation of Unitaries (QET-U)

[Dong, Lin, Tong 2022]



✅ Coherently prepares $f(U)|\psi\rangle$

⚡ Phases φ_i determine $f(\cdot)$

Quantum Szegö Quadrature (QSQ)

Optimal quadrature on the unit circle

Quadrature rule $d \ll N$

$$\langle \psi_0 | f(U) | \psi_0 \rangle \approx \sum_{k=0}^{d-1} \omega_k f(\lambda_k) =: R(f)$$

weights ω_k and nodes λ_k

Quantum Szegö Quadrature (QSQ)

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$$\langle \psi_0 | f(U) | \psi_0 \rangle \approx \sum_{k=0}^{d-1} \omega_k f(\lambda_k) =: R(f)$$

$$U = \sum_n \lambda_n | \phi_n \rangle \langle \phi_n |$$

$$f(U) = \sum_n f(\lambda_n) | \phi_n \rangle \langle \phi_n |$$

$$\langle \psi_0 | f(U) | \psi_0 \rangle = \sum_{k=0}^{N-1} \omega_k f(\lambda_n) =: I(f)$$

$$\omega_k^2 = | \langle \psi_0 | \phi_k \rangle |^2$$

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$$f(U) = \sum_n f(\lambda_n) |\phi_n\rangle\langle\phi_n|$$

$$\langle \psi_0 | f(U) | \psi_0 \rangle = \sum_{k=0}^{N-1} \omega_k f(\lambda_n) =: I(f)$$

$$\omega_k^2 = |\langle \psi_0 | \phi_k \rangle|^2$$

Laurent polynomials

$$f(z) = \sum_{j=-d+1}^{d-1} \alpha_j z^j$$

Szegö quadrature: $R(f)$ exact for degree-$(d-1)$

Riemann-Stieltjes integral

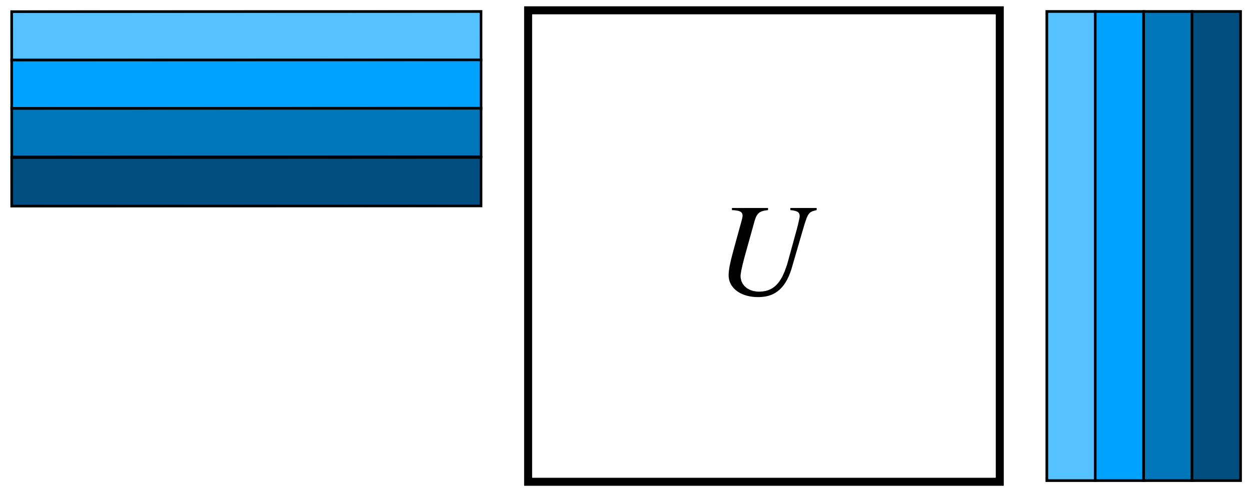
$$I(f) := \int_{\mathbb{T}} f(z) d\mu(z)$$

$$\mu(z) = \sum_{k \in [j]} \omega_k \text{ If } z \in \text{arc}(\lambda_{j-1}, \lambda_j)$$

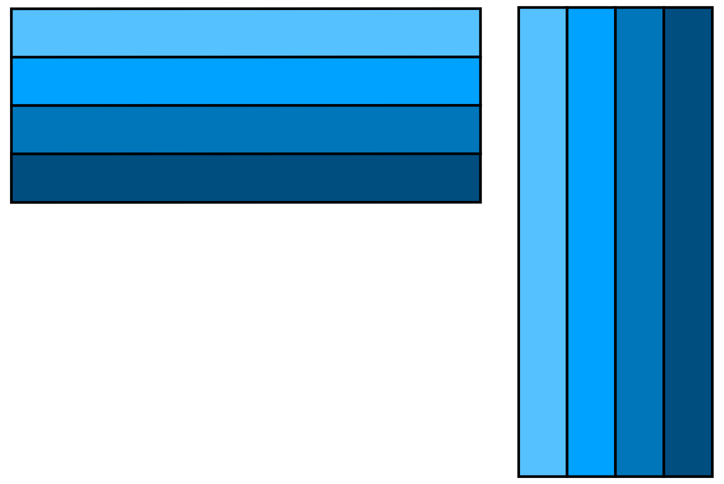
QSQ approximates $I(f)$ using Szegö quadrature rule $R(f)$ with nodes λ_k and weights ω_k computed using the **Quantum Isometric Arnoldi** method

Quantum Isometric Arnoldi

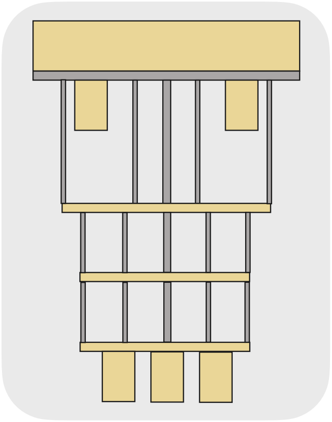
Exact version



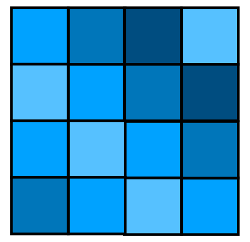
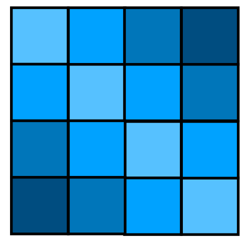
$\langle \psi_i | U | \psi_j \rangle$,



$\langle \psi_i | \psi_j \rangle$



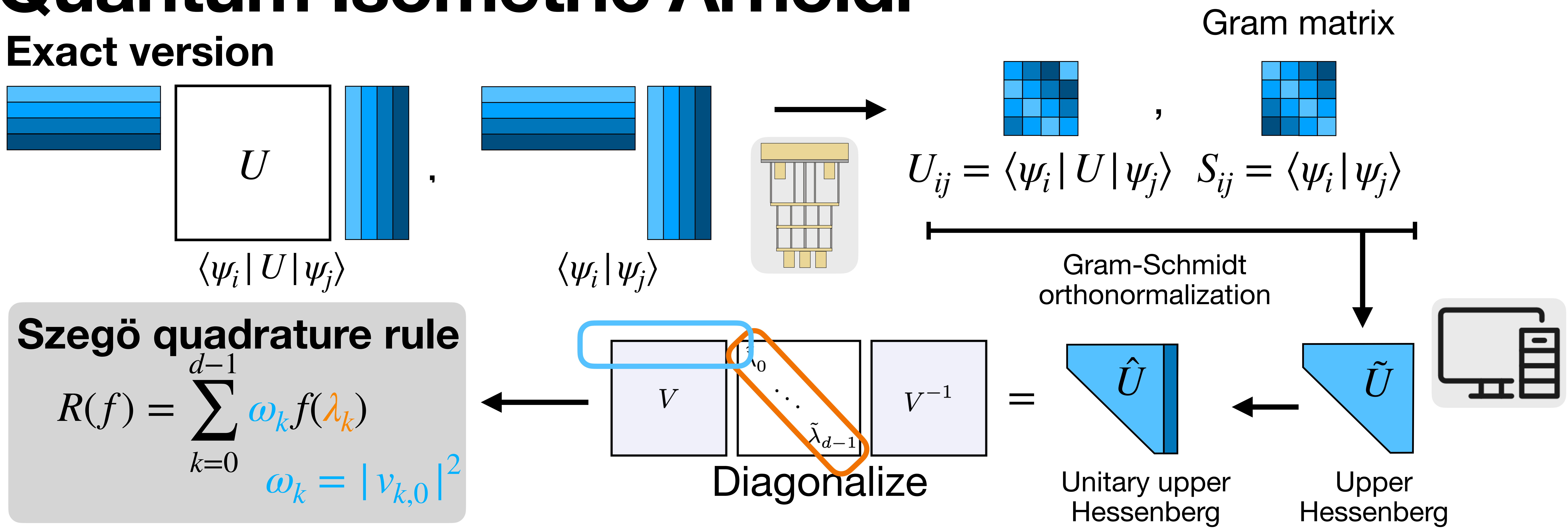
Gram matrix

 , 

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

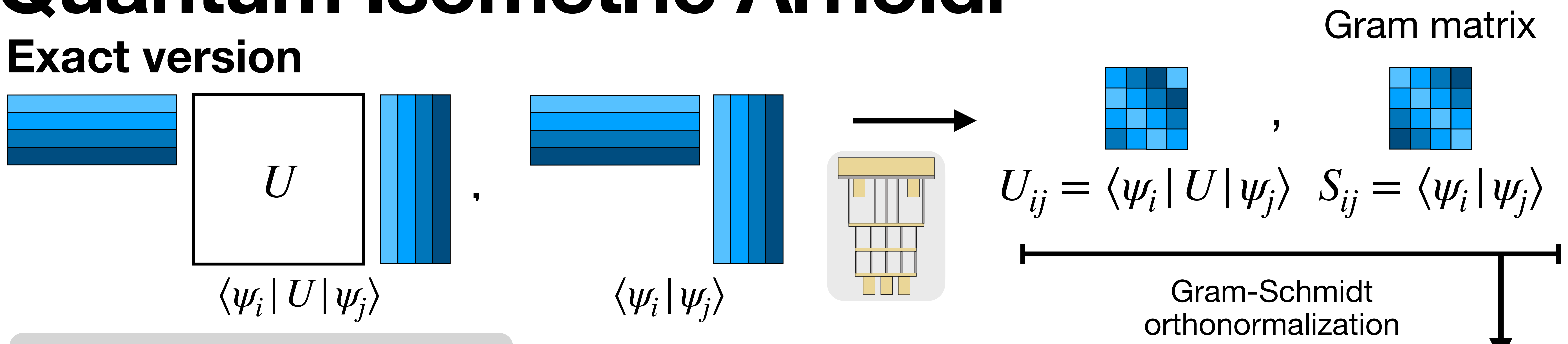
Quantum Isometric Arnoldi

Exact version



Quantum Isometric Arnoldi

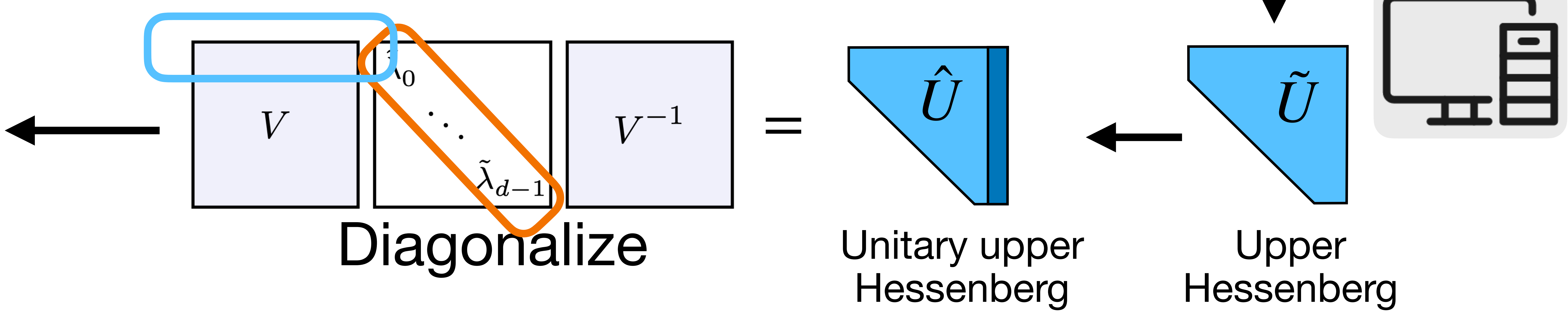
Exact version



Szegö quadrature rule

$$R(f) = \sum_{k=0}^{d-1} \omega_k f(\lambda_k)$$

$$\omega_k = |v_{k,0}|^2$$



Noisy version: Regularization

- Tikhonov regularization on S to mitigate ill-conditioning
- $\hat{U} = PQ^\dagger$ as closest unitary Hessenberg to $\tilde{U} = PDQ^\dagger$

✅ Robust convergence

✅ Evaluate different $f(\,.\,)$ with same data

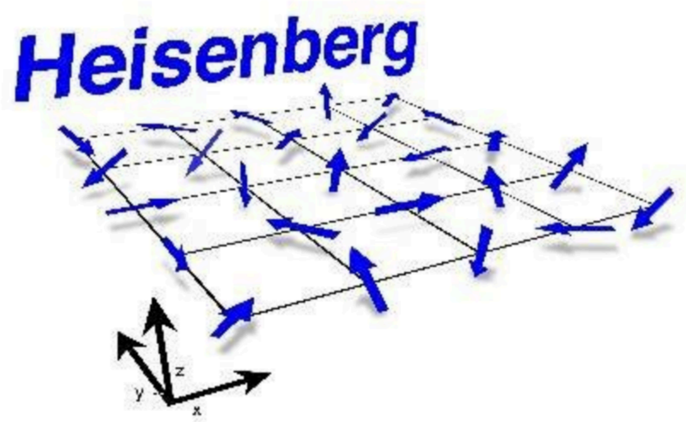
⚡ No coherent access to $f(U)|\psi_0\rangle$

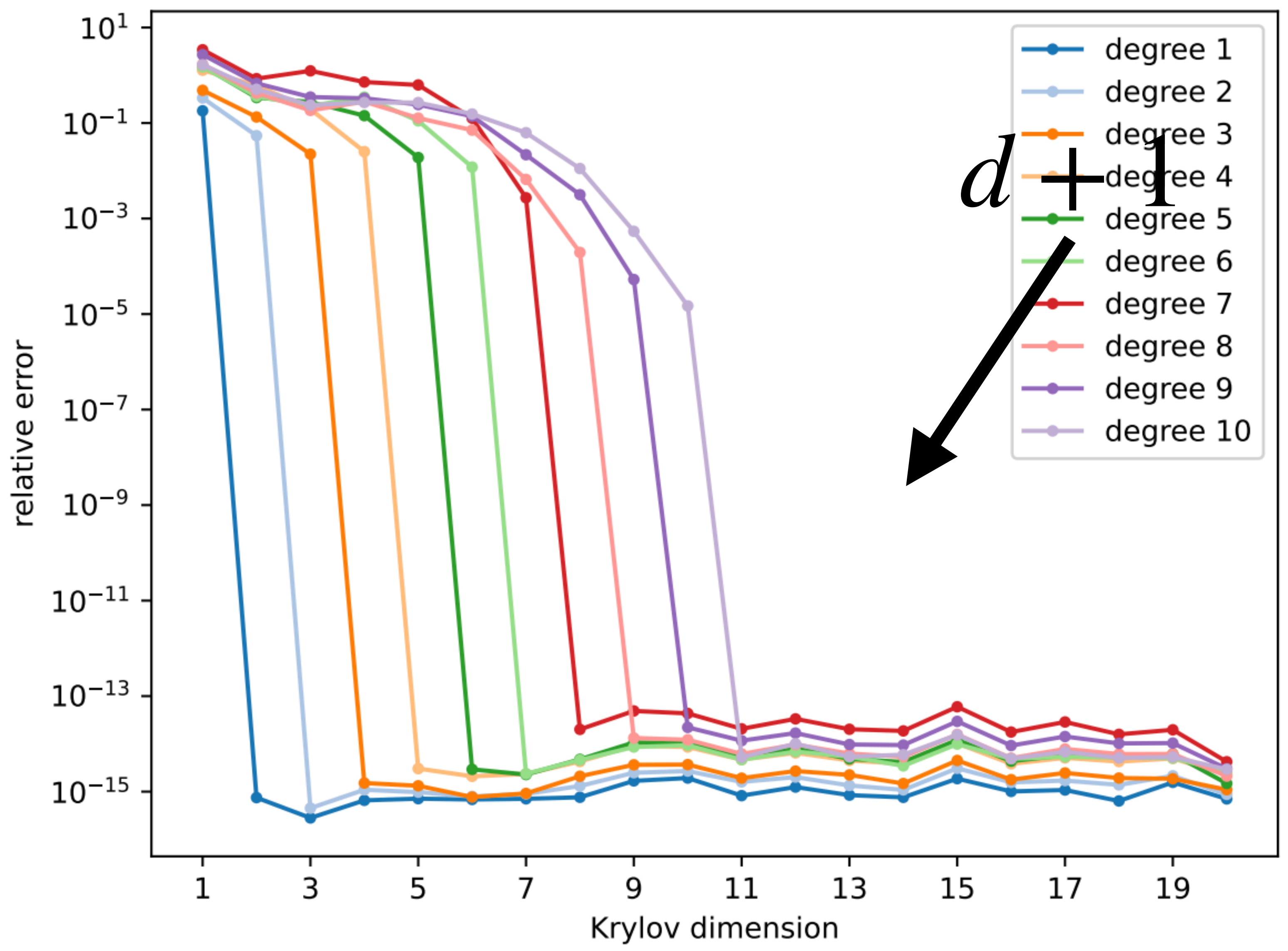
✅ Compute scalar properties $\langle \psi_1 | p(U) | \psi_0 \rangle$

Numerics

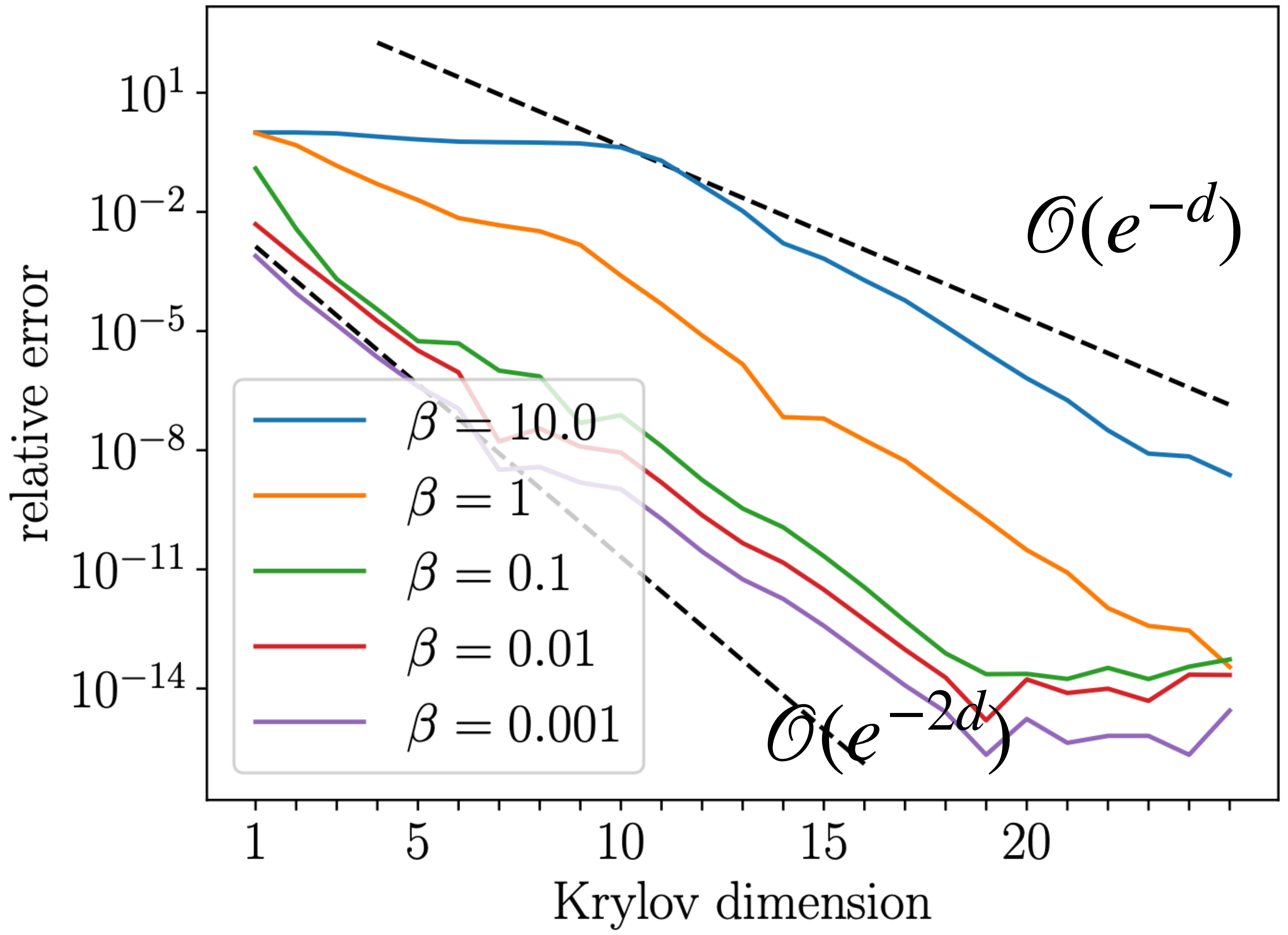
2D XXZ Heisenberg model on 12 sites (4 x 3 lattice)

$U = e^{-\mathrm{i}H\Delta t}$ $\quad |\psi_0\rangle = |1010...10\rangle$ Half-filling antiferromagnetic state



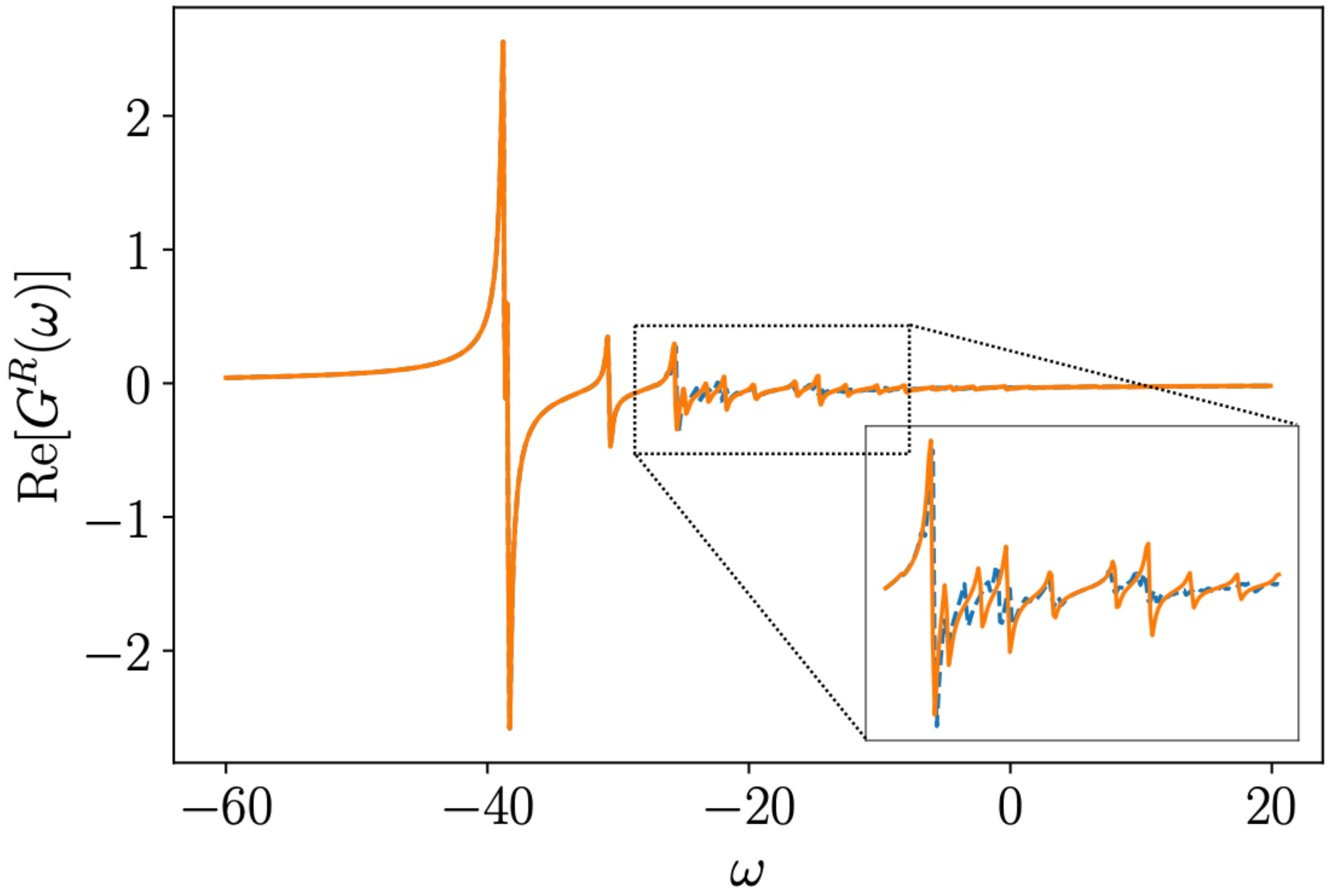


Sanity check:
Random Laurent polynomials



$$\langle \psi_0 | e^{-\beta H} | \psi_0 \rangle = \langle \psi_0 | U^{-\mathrm{i}\beta/\Delta t} | \psi_0 \rangle$$

Gibbs state



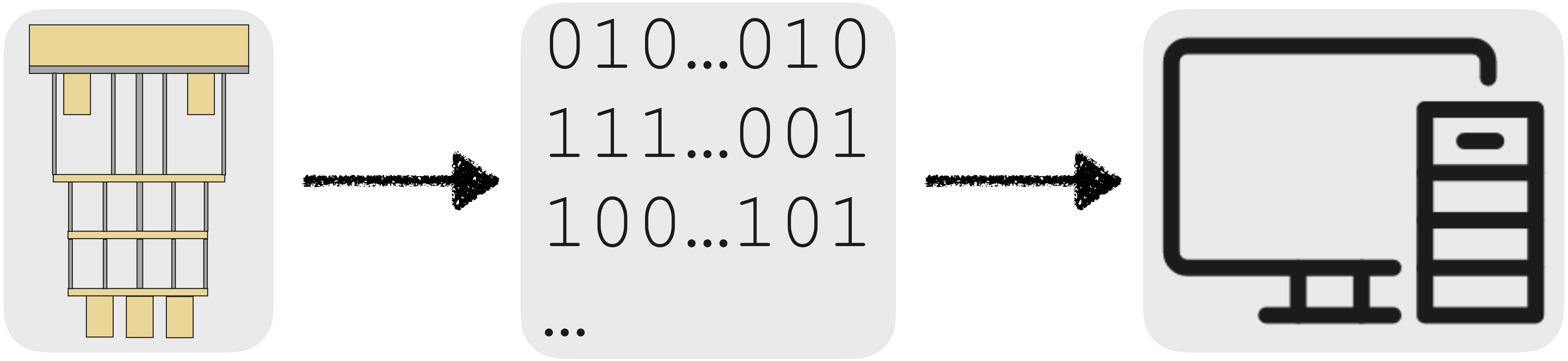
Green's function

Conclusion

- *Measurement-Driven* approaches for **energy estimation** ([M]ODMD) and **matrix functions** (QSQ)
- Classical algorithms based on **subspace** and **signal processing** ideas provide a powerful toolkit to support the quantum computer
- MODMD combines both types of methods with randomized quantum algorithms (shadows) for accurate spectral estimation

Relevant references:

1. ODMD: Shen, Camps, Szasz, Darbha, Klymko, Williams-Young, Tubman, Van Beeumen, *Quantum*, 2025
2. MODMD: Shen, Buzali, Hu, Klymko, Camps, Yelin, Van Beeumen, *PRX Quantum*, 2026
3. QSQ: Kirby, Shen, Camps, Chowdhury, Klymko, Van Beeumen, arXiv:2509.19195



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