

A Quantum Krylov Algorithm for Szegő Quadrature

Will Kirby

¹IBM Quantum

william.kirby@ibm.com

joint work with: Roel van Beeumen², Daan Camps²,
Anirban Chowdhury¹, Katherine Klymko², and Yizhi
Shen²

²Lawrence Berkeley National Laboratory

... preprint coming soon!

Overview

Goal: estimate quantities of the form

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

on a quantum computer.

Inputs for quantum algorithm:

$|\psi\rangle$ = some efficiently preparable state

U = some efficiently implementable unitary

Inputs for classical post-processing:

f = some function

Quantum Krylov algorithms

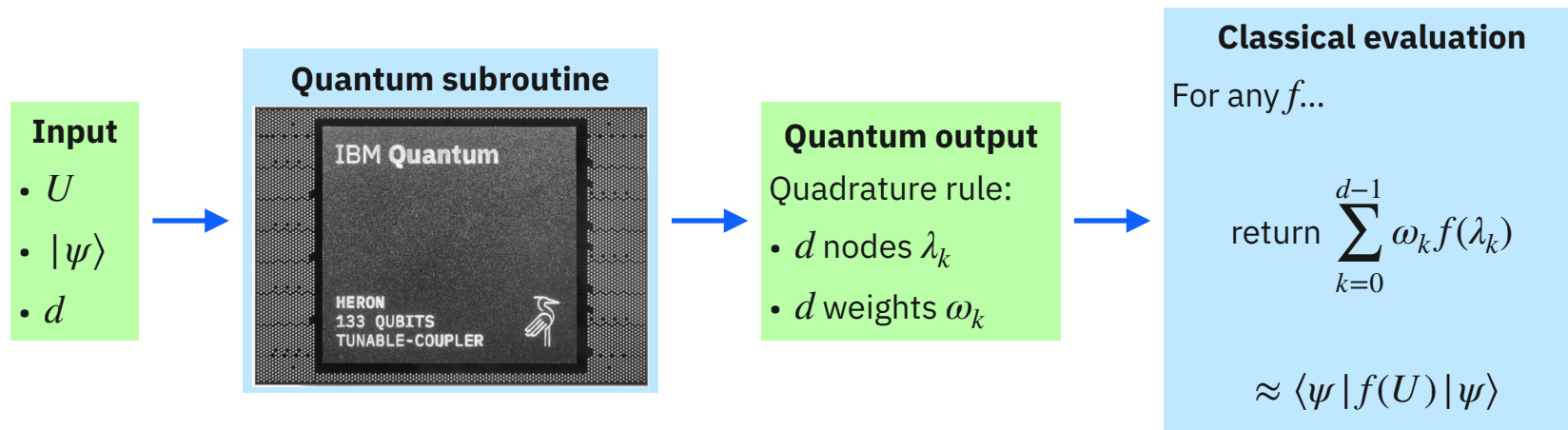
So far, mostly estimating ground state energies

“Quantum version of Lanczos method”

Goal is to apply to large quantum systems,
i.e., exponential-dimension matrices

We extend to estimating functions as on left

Algorithm sketch



Why “quadrature rule”?

Generic quadrature rule: $\int_{\chi} f(x) d\mu(x) \approx \sum_{k=0}^{d-1} \omega_k f(\lambda_k)$

“Optimal” quadrature rules:

- For $\chi =$ real interval, “Gauss quadrature”: d nodes $\Rightarrow$ exact for polynomials up to degree $2d - 1$
- For $\chi = \mathbb{T} =$ unit circle, “Szegő quadrature”: d nodes $\Rightarrow$ exact for Laurent polynomials up to degree $d - 1$


$$f(x) = \sum_{k=-d+1}^{d-1} \alpha_k x^k$$

Where does the integral come from?

Let $|\psi\rangle = \sum_{j=0}^{N-1} \gamma_j |\zeta_j\rangle$ for $|\zeta_j\rangle$ eigenvectors of U

Then $\langle\psi|f(U)|\psi\rangle = \sum_{j=0}^{N-1} |\gamma_j|^2 f(\zeta_j) = \int_{\mathbb{T}} f(z) d\mu(z)$ for $d\mu(z) = \sum_{j=0}^{N-1} |\gamma_j|^2 \delta(z - \zeta_j)$

So the idea of our algorithm, “quantum Szegő quadrature,” is to approximate the expectation value $\langle\psi|f(U)|\psi\rangle$ by approximating the above integral using a Szegő quadrature rule whose nodes and weights we calculate using the quantum computer.

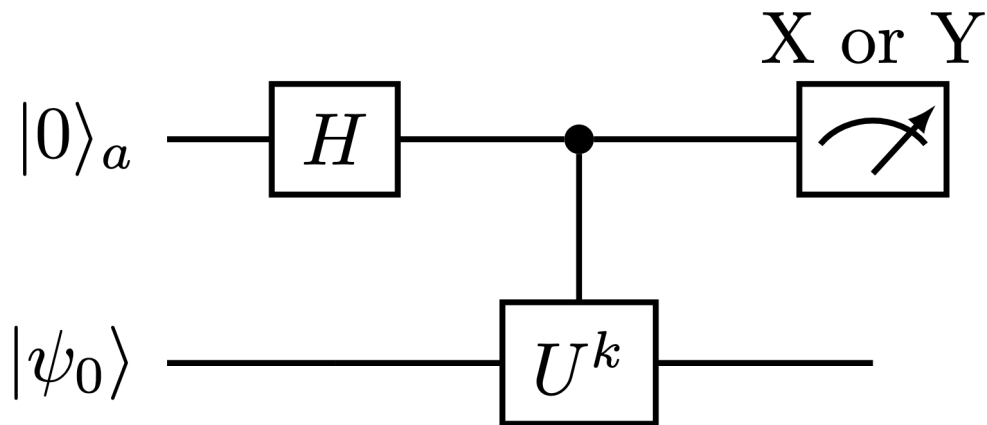
Quantum subroutine: quantum Arnoldi's method

- Ideally, would like Arnoldi's method on $U, |\psi\rangle$
- **Problem:** orthonormalization expensive on quantum
- **Resolution:** don't orthonormalize — form matrix pencil $(\mathbf{U}, \mathbf{S})$ projecting U into Krylov space

$$\mathbf{U} = V^\dagger U V, \quad \mathbf{S} = V^\dagger V \quad \text{for } V = [|\psi\rangle, U|\psi\rangle, U^2|\psi\rangle, \dots, U^{d-1}|\psi\rangle]$$

1. Approximate $(\mathbf{U}, \mathbf{S})$ on quantum computer using Hadamard test or equivalent
2. Classically Gram-Schmidt orthonormalize basis for $\mathbf{U}$ using Gram matrix $\mathbf{S}$ *
3. Formally, result is same upper-Hessenberg $\mathcal{H}$ as from Arnoldi

Aside: Hadamard test



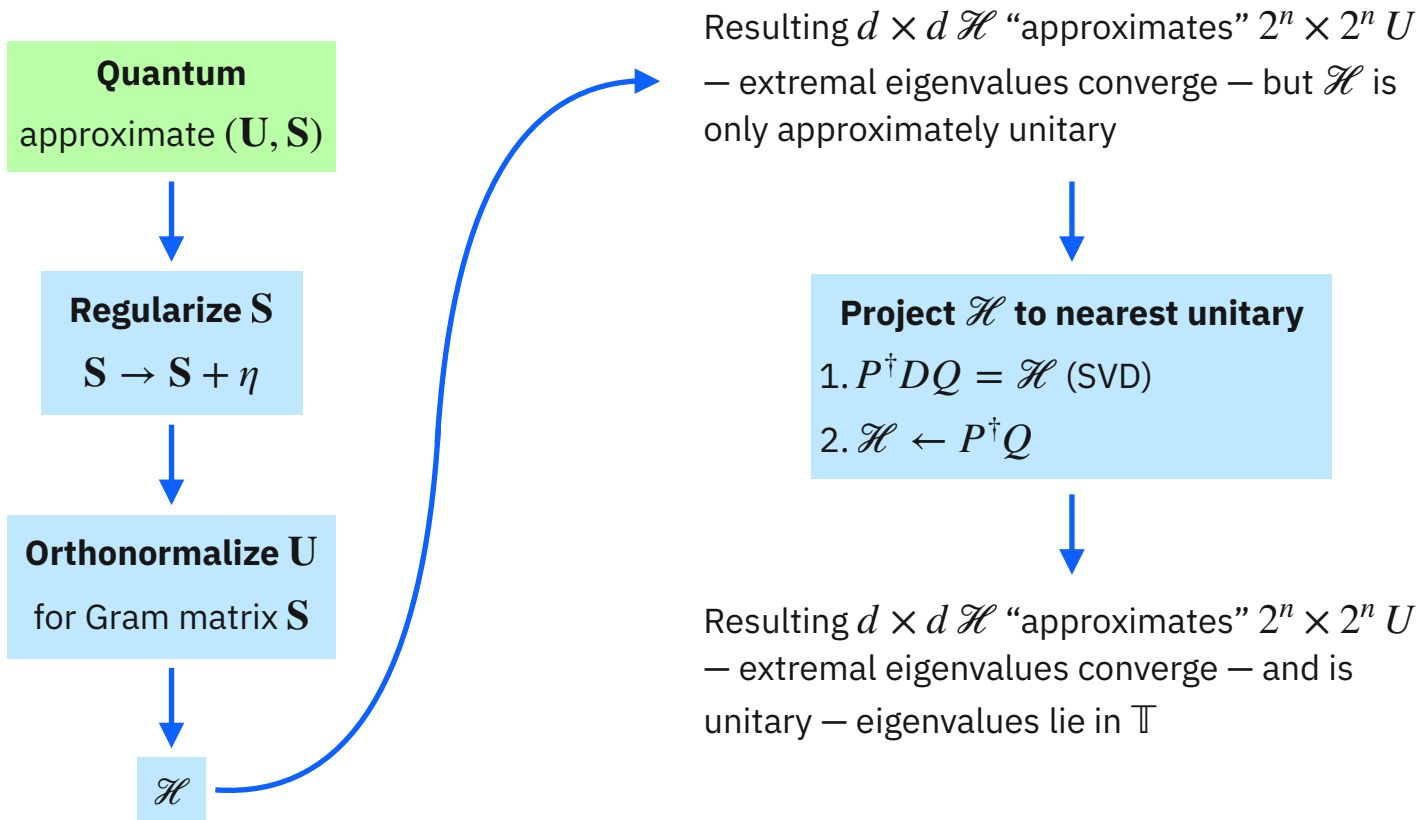
Can show:

$$\langle X \rangle = \text{Re}[\langle \psi | U^k | \psi \rangle], \quad \langle Y \rangle = \text{Im}[\langle \psi | U^k | \psi \rangle]$$

$$\text{so } \langle \psi | U^k | \psi \rangle = \langle X \rangle + i\langle Y \rangle$$

$$\mathbf{U}_{ij} = \langle \psi | U^{j-i+1} | \psi \rangle, \quad \mathbf{S}_{ij} = \langle \psi | U^{j-i} | \psi \rangle$$

Quantum Arnoldi's method* part 2



Quantum Szegő Quadrature

- From slide 5: $\langle \psi | f(U) | \psi \rangle = \int_{\mathbb{T}} f(z) d\mu(z)$
- From slide 8: Quantum isometric Arnoldi $\Rightarrow d \times d \mathcal{H}$ with eigenvalues in $\mathbb{T}$ (complex unit circle)
- Let $\lambda_k, v_k =$ eigenvalues, eigenvectors of $\mathcal{H}^T$

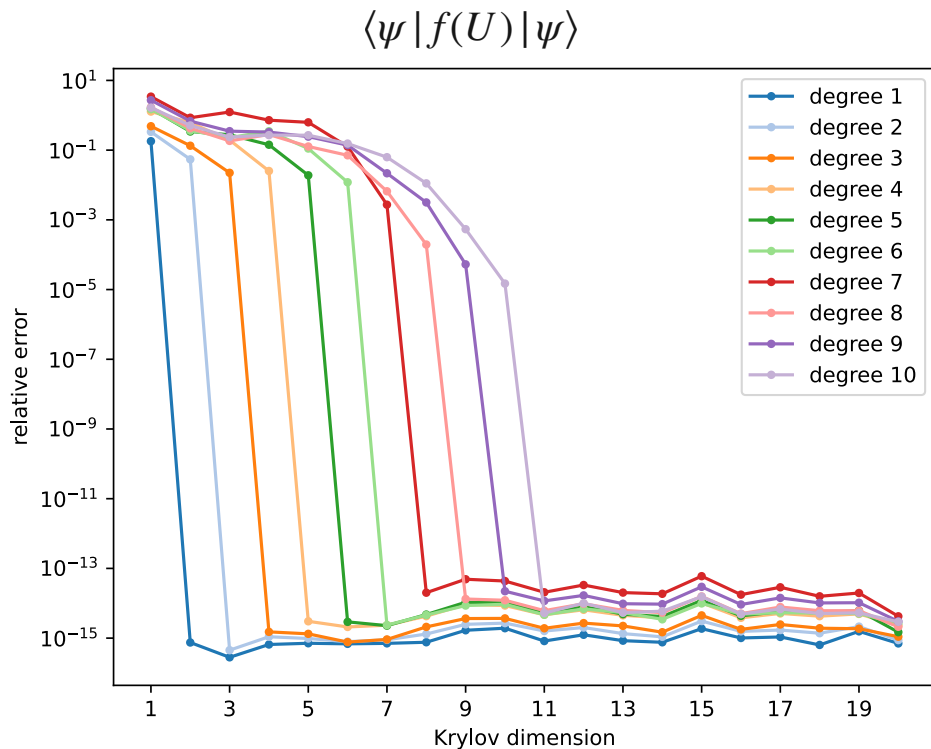
Can prove: a Szegő quadrature rule for the integral above is

$$\int_{\mathbb{T}} f(z) d\mu(z) = \sum_{k=0}^{d-1} |v_{k,0}|^2 f(\lambda_k)$$



zeroth entry in v_k

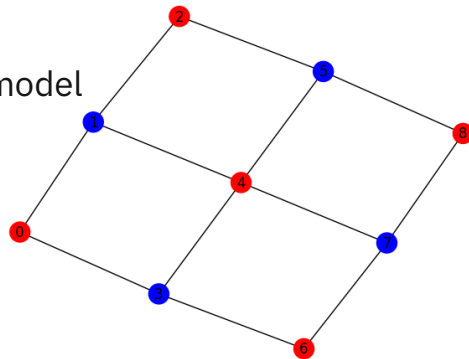
Numerical illustrations part 1



- System: Heisenberg model

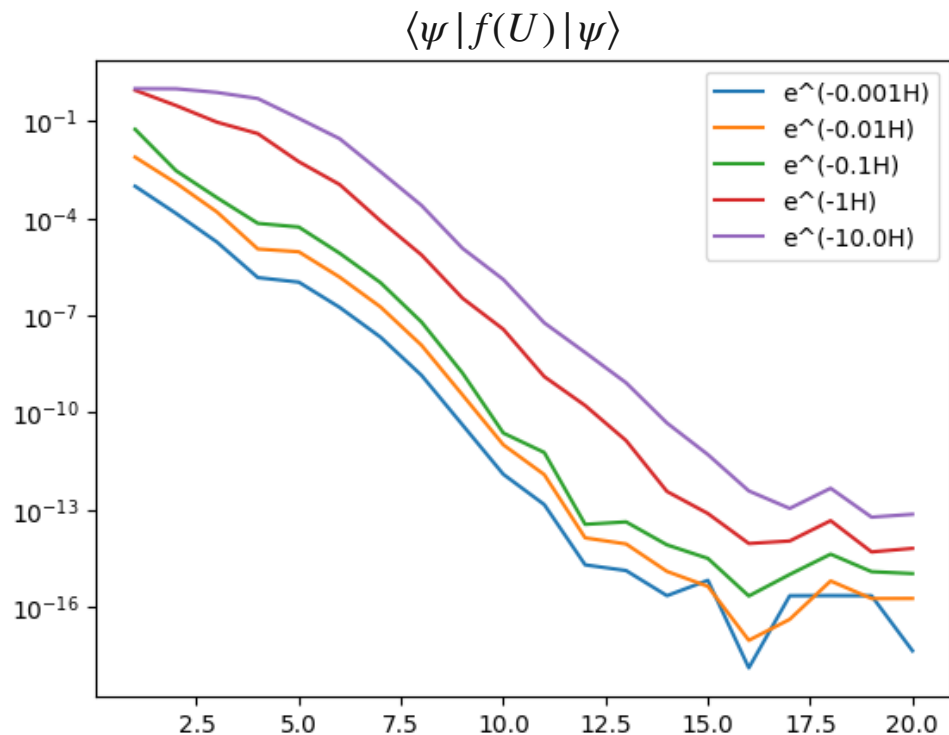
- State:

$$|\psi\rangle =$$



- Classically simulate quantum Szegő quadrature
- f = random Laurent polynomials
- Points in plot = mean errors over 10 instances

Numerical illustrations part 2

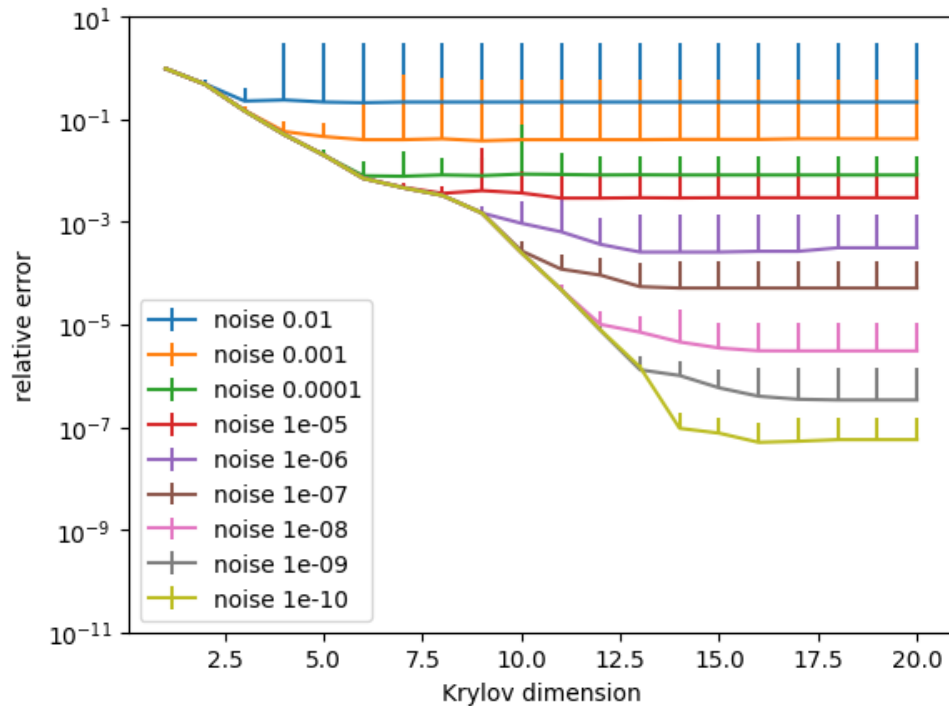


- Same system and state
- Classically simulate quantum Szegő quadrature
- $f(U) = U^{i\beta/\Delta t} = e^{-\beta H} \quad (U = e^{-iH\Delta t})$

There is a known approximation of $e^{-\beta H}$ as a polynomial in U , which also converges exponentially, but it is tens of orders of magnitude worse than these results.

Numerical illustrations part 3

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



- Same system and state
- Classically simulate quantum Szegő quadrature
- $f(U) = U^{i\beta/\Delta t} = e^{-\beta H} \quad (U = e^{-iH\Delta t})$
- Set $\beta = 1$, vary noise rate on matrix elements

How to think about this tool?

Uses same data as other quantum Krylov algorithms

Like quantum signal processing* or QET-U*, evaluates functions of operators on Hilbert space

Upsides:

- Does not require knowing function beforehand
 - Can calculate quadrature rule, then use for any function
- Does not require calculating explicit Laurent series
- Noise robust

Downside: (so far) only for evaluating expectation values $\langle \psi | f(U) | \psi \rangle$

Thank you!

Questions?



Proof sketch

1. Define $\vec{p}(x) = (p_0(x), p_1(x), \dots, p_{d-1}(x))$ such that orthonormal Krylov basis = $\{p_i(U)v \mid i = 0, \dots, d-1\}$
2. Define *para-orthogonal polynomials* $\tilde{p}_j(x) = p_j(x) + \tau x^j \bar{p}_j(x^{-1})$, $|\tau| = 1$
3. Eigenvalues λ_k of $\mathcal{H}^T$ are zeros of $\tilde{p}_d$, and $\vec{p}(\lambda_k)$ are corresponding eigenvectors *
4. Zeros of $\tilde{p}_d$ are nodes of Szegő quadrature rule *
5. Weights are $\omega_k = \frac{1}{\|\vec{p}(\lambda_k)\|^2}$ (following **, two applications of Christoffel-Darboux for complex unit circle)
6. If v_k is normalized eigenvector of $\mathcal{H}^T$, $\|\vec{\phi}(\lambda_k)\| = \frac{\|\vec{\phi}(\lambda_k)\|}{\|\vec{v}_k\|} = \frac{|\phi_0(\lambda_k)|}{|v_{k,0}|} = \frac{1}{|v_{k,0}|}$

* W. B. Jones, O. Njåstad, and W. J. Thron, Bulletin of the London Mathematical Society, vol. 21, no. 2, pp. 113–152, 1989.

* W. B. Gragg, Journal of Computational and Applied Mathematics, vol. 46, no. 1, pp. 183–198, 1993.

** Section 2.9 in H. S. Wilf, Mathematics for the Physical Sciences Dover Publications Inc., New York, NY, 1962.