CS 59300 – Algorithms for Data Science

Classical and Quantum approaches

Lecture 15 (10/30)

Quantum eigenvalue problems (II)

https://ruizhezhang.com/course_fall_2025.html

Part of the slides are borrowed from Zhiyan Ding's talk

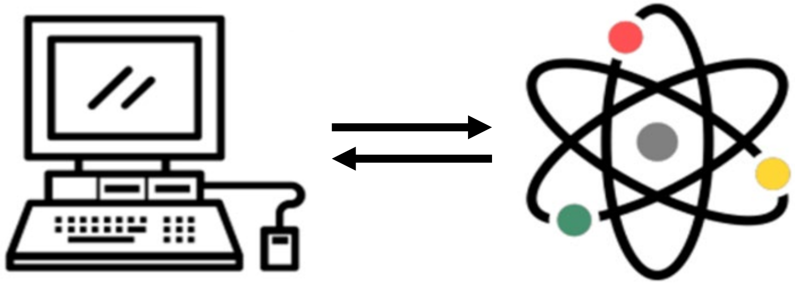
Two different approaches

	Heisenberg limit	Allow $p_0 < 1$	#ancilla	Circuit depth
Hadamard test	✗	✗	1	Short
Kitaev's QPE	✓	✓	Many	Long

Can we design an algorithm with all these good properties?

Early fault-tolerant (EFT) phase estimation

- Post-Kitaev type: (Lin-Tong ’22; Dong et al. ’22; **Z.** et al. ’22; Ding-Lin ’23; Wang et al. ’23; Ni et al. ’23; Ding et al. ’24; Yi et al. ’24; Castaldo-Corni ’25…)
- Quantum Krylov subspace type: (Parrish-McMahon ’19; Stair et al. ’20; Epperly et al. ’22; Klymko et al. ’22; Shen et al. ’23; Li et al. ’23; Ding et al. ’24...)
- Experimental relevance: (Blunt et al. ’23; Kiss et al. ’24…)



Unified framework

1 Generate a grid $\{t_i\}_{i=1}^{N_S} \subset \mathbb{R}$

2 Run Hadamard tests with evolution times $\{t_i\}_{i=1}^{N_S}$

3 Classically post-process the dataset $\{(t_i, Z_i)\}_{i=1}^{N_S}$

RPE (with exact ground state):

An exponential grid:

$$\left\{1, \frac{3}{2}, \left(\frac{3}{2}\right)^2, \left(\frac{3}{2}\right)^3, \dots, \mathcal{O}(\epsilon^{-1})\right\}^{\times \mathcal{O}(1)}$$

- $T_{\max} = \mathcal{O}(\epsilon^{-1})$
- $T_{\text{total}} = \mathcal{O}(\epsilon^{-1})$

Shrinking the confidence interval

QPE:

An exponential grid:

$$\{1, 2, 2^2, 2^3, \dots, \mathcal{O}(p_0^{-1}\epsilon^{-1})\}^{\times p_0^{-1}}$$

Single-shot for the whole grid

- $T_{\max} = \mathcal{O}(p_0^{-1}\epsilon^{-1})$
- $T_{\text{total}} = \mathcal{O}(p_0^{-2}\epsilon^{-1})$

n/a

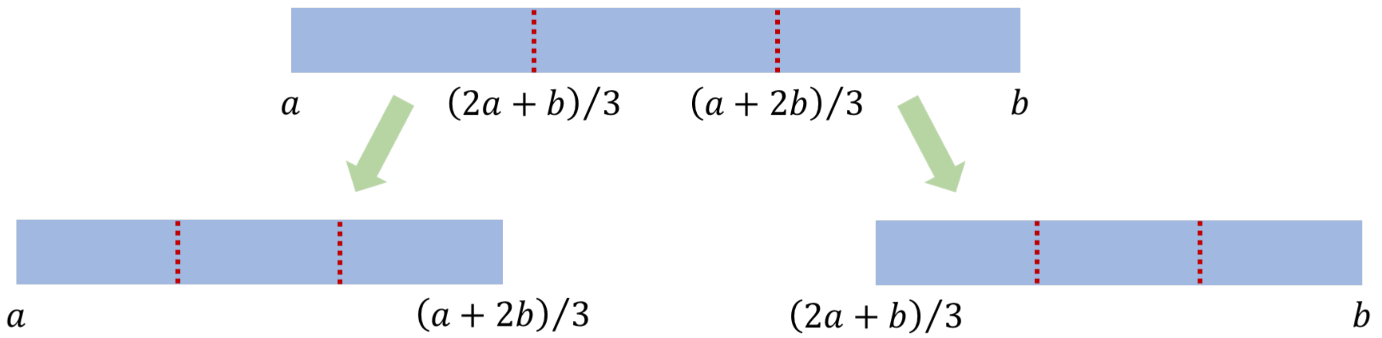
Post-Kitaev phase estimation

1. Robust phase estimation
2. Optimization
3. Filtering
4. (Classical super-resolution methods)

Robust phase estimation: algorithm

Suppose we know $a \leq -\lambda_0 \leq b$. We want to determine

1. $a \leq -\lambda_0 \leq \frac{a+2b}{3}$
2. $\frac{2a+b}{3} \leq -\lambda_0 \leq b$



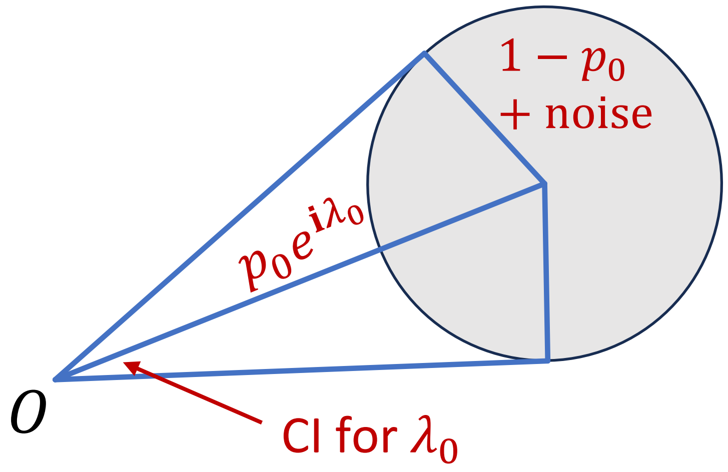
- If we can do that then we can reduce the uncertainty by $1/3$ at each step
- $\mathcal{O}(\log(\epsilon^{-1}))$ iterations are needed for ϵ precision

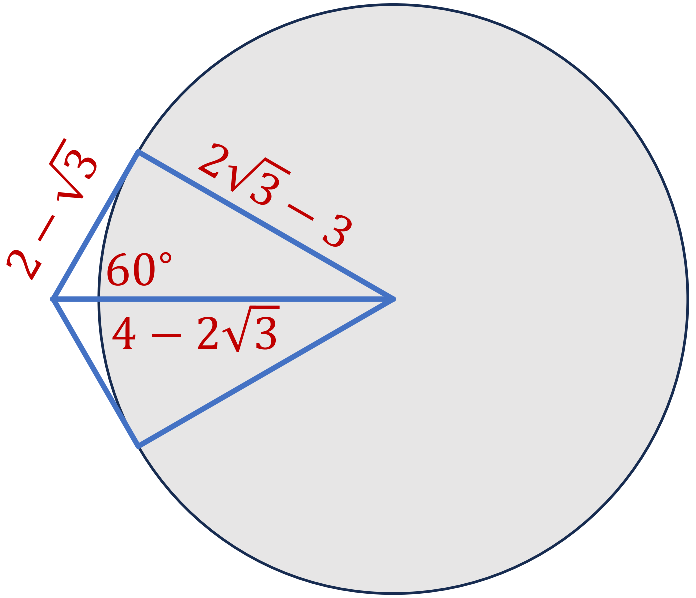
Robust phase estimation

Theorem (Ni-Li-Ying ’23). Suppose $|\phi\rangle = \sum_k c_k |E_k\rangle$ and let $p_0 \coloneqq |c_0|^2 > 4 - 2\sqrt{3} \approx 0.536$. Then, there is an algorithm that achieves

$$\Pr\left[\left|\hat{\lambda} - \lambda_0\right|_{2\pi} < \frac{\pi}{3}\epsilon\right] > 1 - \delta$$

using $T_{\max} = \mathcal{O}(\epsilon^{-1})$ and $T_{\text{total}} = \mathcal{O}\left(\epsilon^{-1}(\log \delta^{-1} + \log\log \epsilon^{-1})\right)$





When $p_0 > 4 - 2\sqrt{3}$, λ_0 can be estimated with CI $= 2 \cdot \frac{\pi}{3} = \frac{2\pi}{3}$

Robust phase estimation: improved algorithm

- $J \leftarrow \log(\epsilon^{-1})$ and $N_S \leftarrow \Theta(\log(\delta^{-1}) + \log\log(\epsilon^{-1}))$
- **For** $j = 0,1,\dots,J$ **do**
  - $t_j \leftarrow 2^j$ (an exponential grid)
  - Run the Hadamard test circuits for N_S times to obtain $\overline{Z}_j$, an estimate of $\langle\phi|e^{\mathbf{i}2^j H}|\phi\rangle$
  - Define a candidate set $\mathcal{S}_j \coloneqq \left\{\frac{2k\pi+\arg\overline{Z}_j}{2^j}\right\}_{k=0,\dots,2^j-1}$
  - $\theta_j \leftarrow \arg\min_{\theta\in\mathcal{S}_j} \left|\theta - \theta_{j-1}\right|_{2\pi}$
- Output θ_J

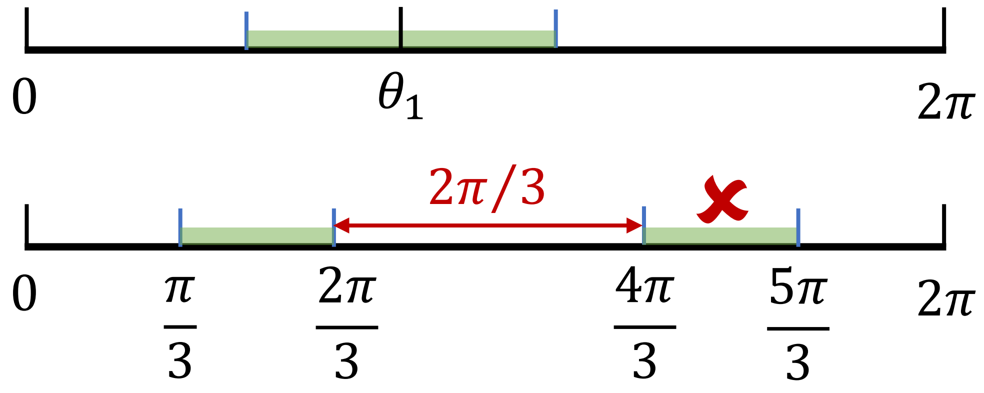
Robust phase estimation: refined analysis

Iteration 1:

- $\langle\phi|e^{\mathbf{i}H}|\phi\rangle$, estimate λ_0 with CI $= \frac{2\pi}{3}$ by the assumption on p_0

Iteration 2:

- $\langle\phi|e^{\mathbf{i}2H}|\phi\rangle$, estimate $2\lambda_0$ with CI $= \frac{2\pi}{3}$
- Aliasing effect: 2 possible sub-CIs
  - Suppose $\arg \overline{Z}_2 = \pi$ and $2\lambda_0 \in \left(\frac{2\pi}{3}, \frac{4\pi}{3}\right)$
  - One CI for λ_0 is $\left(\frac{\pi}{3}, \frac{2\pi}{3}\right)$
  - Another CI is $\left(\left(\frac{2\pi}{3}+2\pi\right)/2, \left(\frac{4\pi}{3}+2\pi\right)/2\right) = \left(\frac{4\pi}{3}, \frac{5\pi}{3}\right)$



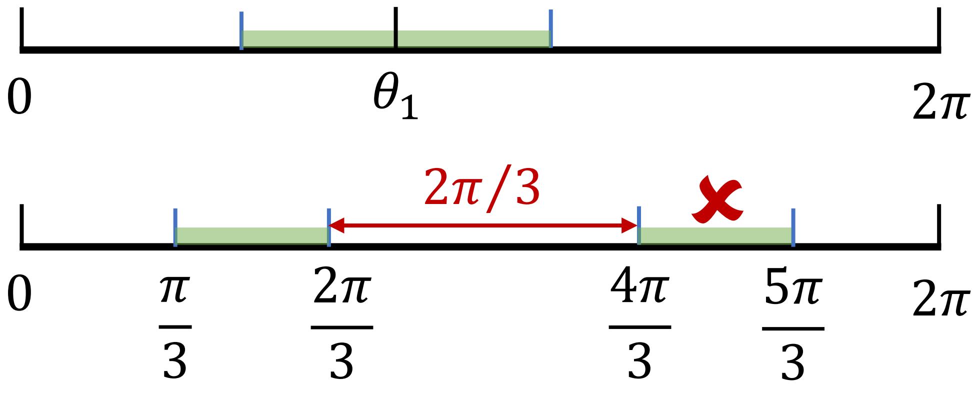
Robust phase estimation: refined analysis

Iteration 1:

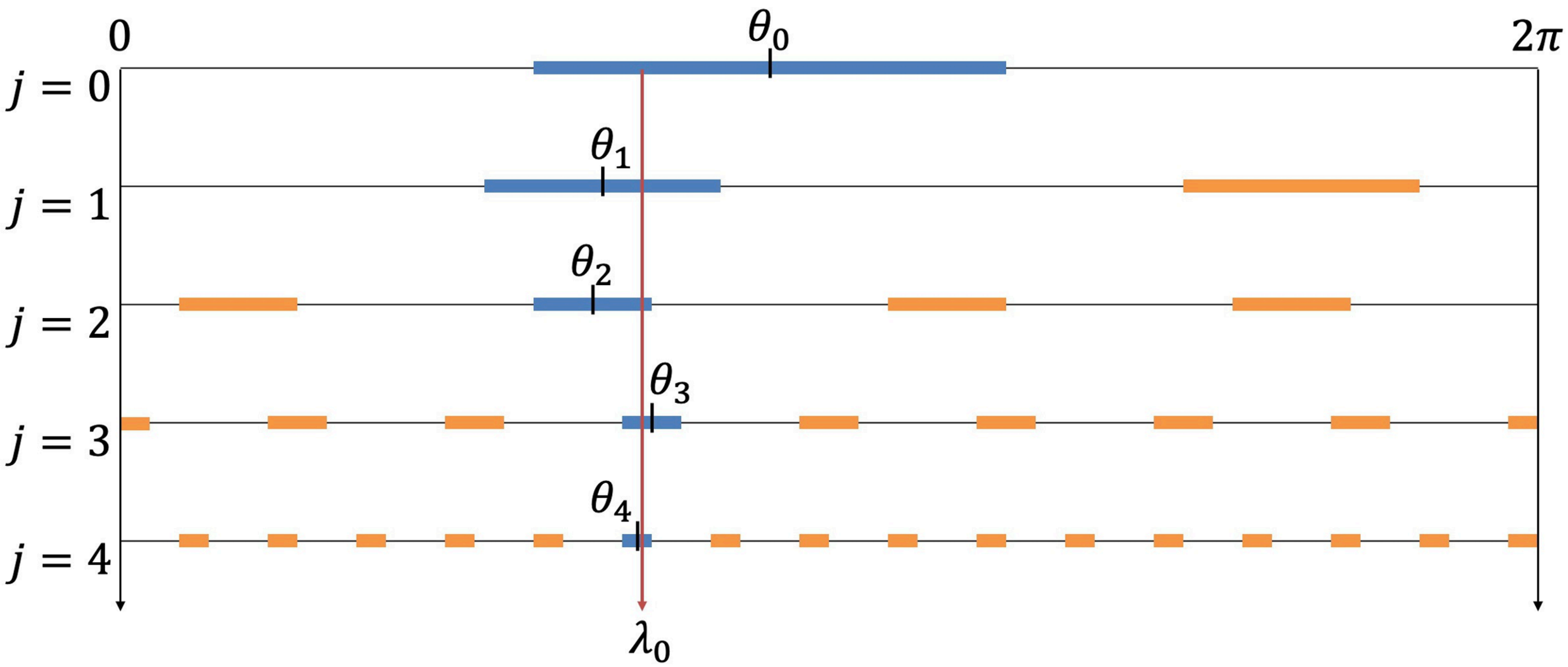
- $\langle\phi|e^{\mathbf{i}H}|\phi\rangle$, estimate λ_0 with CI $= \frac{2\pi}{3}$ by the assumption on p_0

Iteration 2:

- $\langle\phi|e^{\mathbf{i}2H}|\phi\rangle$, estimate $2\lambda_0$ with CI $= \frac{2\pi}{3}$
- Aliasing effect: 2 possible sub-CIs
- CI for $\langle\phi|e^{\mathbf{i}H}|\phi\rangle \leq \frac{2\pi}{3}$ ensures only 1 sub-CI intersects
- So, we can discard the ghost ones



Robust phase estimation: refined analysis



- For ϵ precision, we need $\log(\epsilon^{-1})$ iterations
- The j-th iteration's cost is $2^j \times N_s = \tilde{O}(2^j)$. Hence, the total evolution time is $\tilde{O}(\epsilon^{-1})$
- The maximal evolution time is $2^{\log \epsilon^{-1}} = \epsilon^{-1}$

Proof of the shrinking confidence intervals

Lemma. Let $p_0 < 4 - 2\sqrt{3}$, and define the noise-level $\alpha(p_0)$ as:

$$\alpha(p_0) \coloneqq \frac{\sqrt{3}}{2} p_0 - (1 - p_0) > 0$$

If $\left|\overline{Z}_j - \langle\phi|e^{\mathbf{i}2^j H}|\phi\rangle\right| < \alpha(p_0)$, then

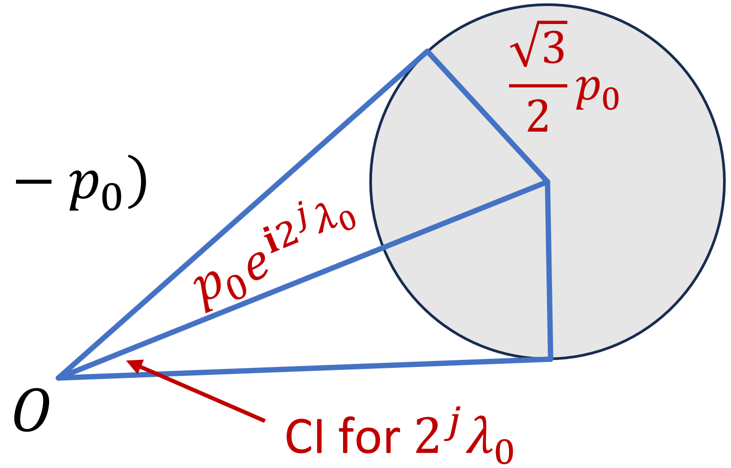
$$2^j \lambda_0 \in \left(\arg \overline{Z}_j - \frac{\pi}{3}, \arg \overline{Z}_j + \frac{\pi}{3}\right) \mod 2\pi$$

Proof.

$$\begin{aligned}\alpha(p_0) &> \left|\overline{Z}_j - \langle\phi|e^{\mathbf{i}2^j H}|\phi\rangle\right| = \left|\overline{Z}_j - p_0 e^{i2^j\lambda_0} - \text{residue}\right| \\ &\geq \left|\overline{Z}_j - p_0 e^{i2^j\lambda_0}\right| - |\text{residue}| \geq \left|\overline{Z}_j - p_0 e^{i2^j\lambda_0}\right| - (1 - p_0)\end{aligned}$$

- The CI for $2^j\lambda_0$ is $2 \cdot \arcsin\frac{\sqrt{3}}{2} = \frac{2\pi}{3}$

$\blacksquare$



Unified framework

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3 Classically post-process the dataset $\{(t_i, Z_i)\}_{i=1}^{N_S}$

RPE (improved):

An exponential grid:

$\{1,2,2^2,2^3,\dots,\epsilon^{-1}\}^{\times\tilde{\mathcal{O}}(1)}$

- $T_{\max} = \mathcal{O}(\epsilon^{-1})$
- $T_{\text{total}} = \mathcal{O}(\epsilon^{-1})$

Shrinking the CIs

RPE (improved, large p_0):

An exponential grid:

$$\left\{1,2,2^2,2^3,\dots,\frac{1-p_0}{\epsilon}\right\}^{\times(1-p_0)^{-2}}$$

- $T_{\max} = \mathcal{O}\left(\frac{1-p_0}{\epsilon}\right)$
- $T_{\text{total}} = \mathcal{O}\left((1-p_0)^{-1}\epsilon^{-1}\right)$

Shrinking the CIs

Post-Kitaev phase estimation

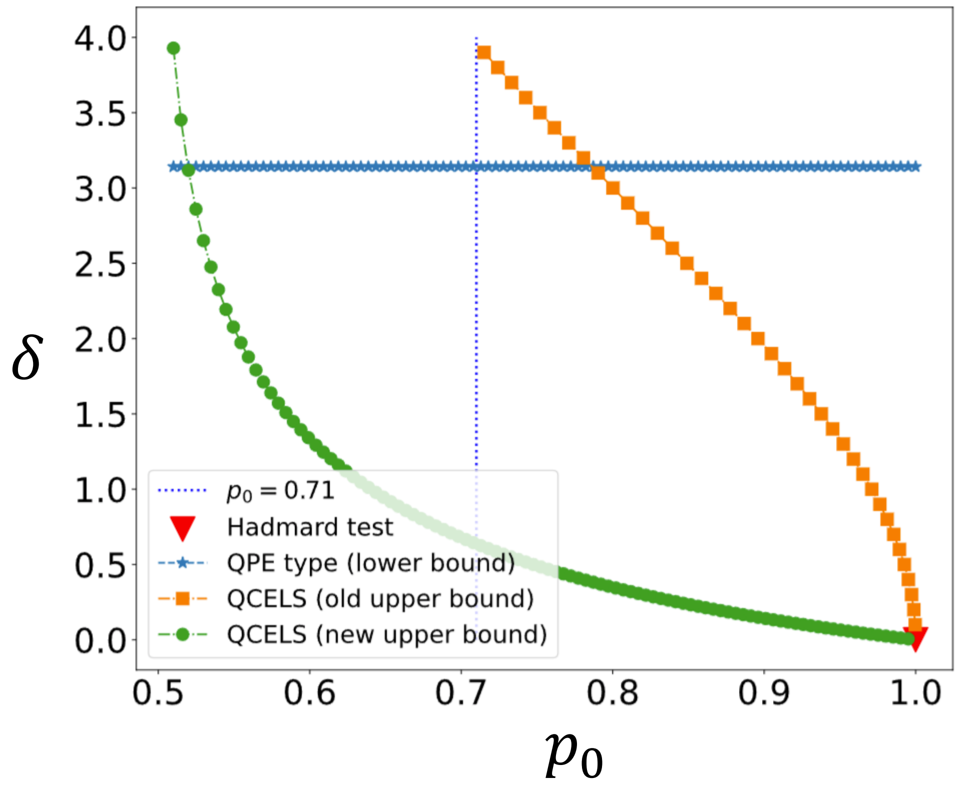
1. Robust phase estimation
2. Optimization
3. Filtering
4. (Classical super-resolution methods)

Quantum complex exponential least squares

Theorem (Ding-Lin ’23). Assume $p_0 > 0.5$. There exists an algorithm (QCELS) such that, with high probability, it outputs $\left|\hat{\lambda} - \lambda_0\right| \leq \epsilon$ with

- Maximal evolution time $T_{\max} = \mathcal{O}\left(\frac{1-p_0}{\epsilon}\right)$
- Total evolution time $T_{\text{total}} = \mathcal{O}\left(\frac{1}{\epsilon}\right)$

$$T_{\max} := \frac{\delta}{\epsilon}$$

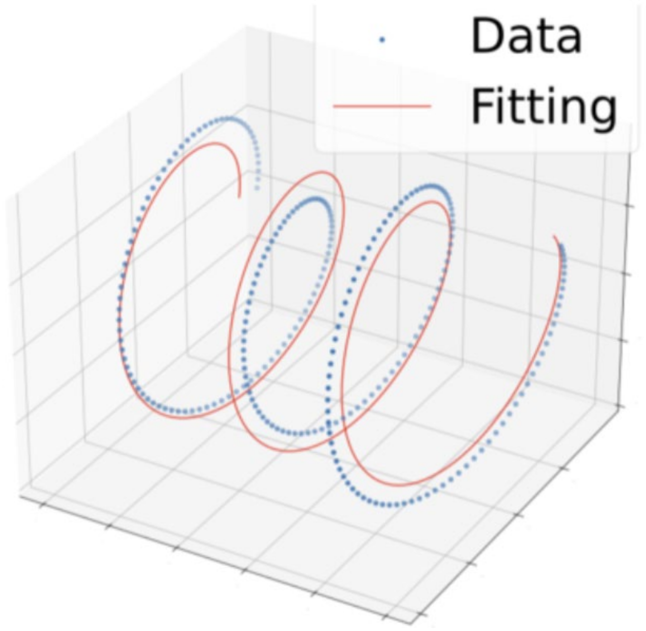


QCELS

- Sample $t_1, \dots, t_{N_S} \sim_{\text{i.i.d.}} \mathcal{N}(0, T^2) \cdot \mathbf{1}_{|t| \le \gamma T}$ i.e. a truncated Gaussian distribution
- For each t_n, run Hadamard test to obtain one sample $Z_n \in \{\pm 1 \pm \mathbf{i}\}$
- Solve the optimization problem:

$$(r^\star, \theta^\star) = \arg\min_{r,\theta} \frac{1}{N_S} \sum_{n=1}^{N_S} \left| Z_{t_n} - r e^{-\mathbf{i}\theta t_n} \right|^2$$

- Output $\theta^\star$



QCELS optimization in the large-N limit

$$(r^\star, \theta^\star) = \arg\min_{r,\theta} \frac{1}{N_S} \sum_{n=1}^{N_S} \left| Z_{t_n} - r e^{-\mathbf{i}\theta t_n} \right|^2 \qquad \text{(QCELS)}$$

$$\Big\downarrow N \to \infty$$

$$(r^\star, \theta^\star) = \arg\min_{r,\theta} \int_{-\gamma T}^{\gamma T} \mathbb{E}\left[\left| Z_t - r e^{-\mathbf{i}\theta t} \right|^2 \right] a(t) \mathrm{d}t$$

Recall $t_n \sim a(t)$

$$= \arg\min_{r,\theta} \int_{-\gamma T}^{\gamma T} \left| \mathbb{E}[Z_t] e^{\mathbf{i}\theta t} - r \right|^2 a(t) \mathrm{d}t$$

Explicitly optimize r: $r^\star = \int_{-\gamma T}^{\gamma T} \mathbb{E}[Z_t] e^{\mathbf{i}\theta t} a(t) \mathrm{d}t$

QCELS optimization in the large-N limit

$$(r^\star,\theta^\star) = \arg\min_{r,\theta} \frac{1}{N_S}\sum_{n=1}^{N_S}\left|Z_{t_n} - re^{-\mathbf{i}\theta t_n}\right|^2 \qquad \text{(QCELS)}$$

$$\Big\downarrow N \to \infty$$

$$\theta^\star = \arg\max_\theta \left|\int_{-\gamma T}^{\gamma T} \mathbb{E}[Z_t] e^{\mathbf{i}\theta t} a(t)\mathrm{d}t\right|^2$$

Recall $\mathbb{E}[Z_t] = \sum_k p_k e^{-\mathbf{i}\lambda_k t}$

$$= \arg\max_\theta \left|\sum_k p_k \int_{-\gamma T}^{\gamma T} e^{\mathbf{i}(\theta-\lambda_k)t} a(t)\mathrm{d}t\right|^2$$

QCELS optimization in the large-N limit

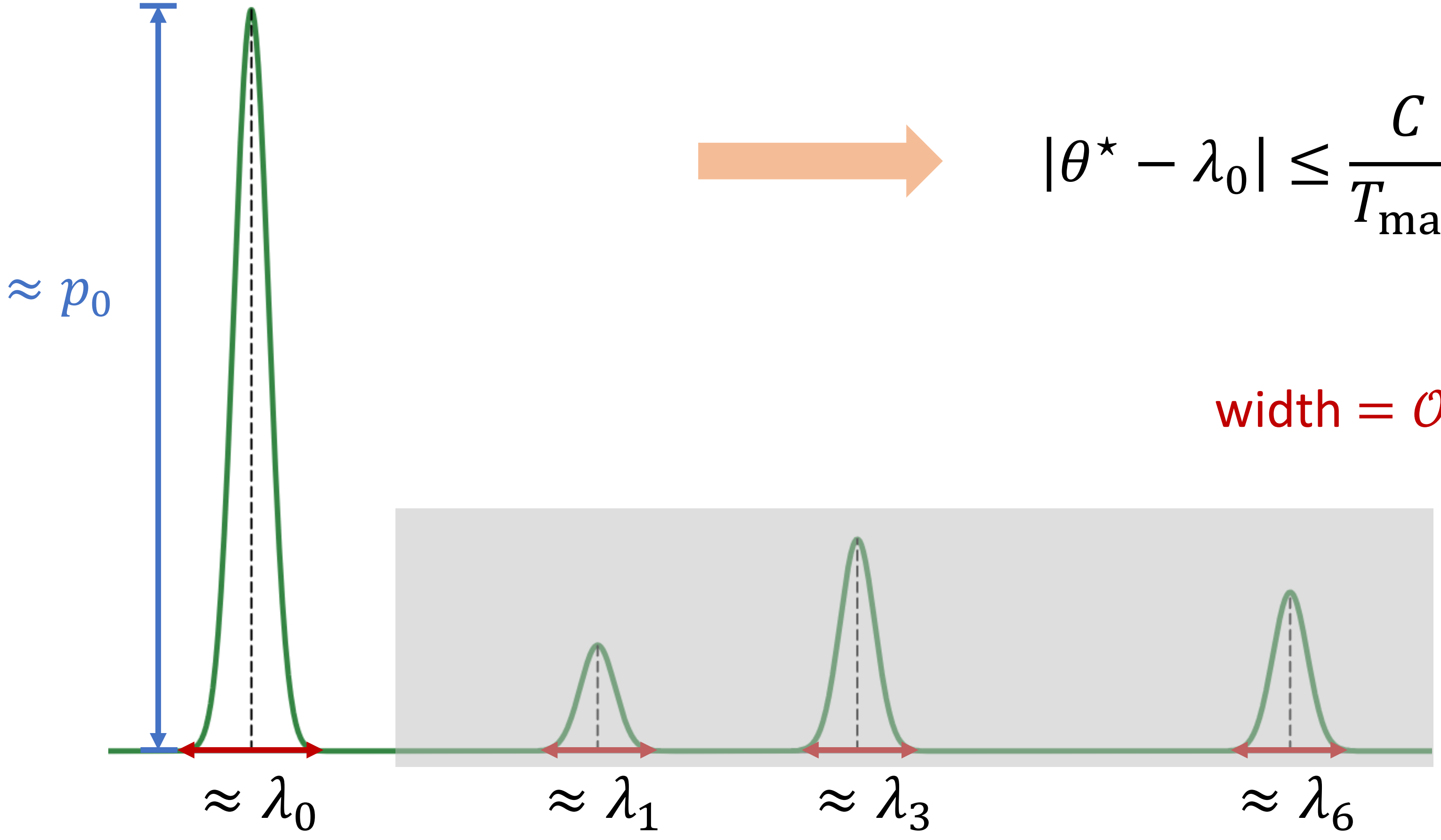
$$\theta^\star = \arg\max_\theta \left| \sum_k p_k \underbrace{\int_{-\gamma T}^{\gamma T} e^{\mathbf{i}(\theta-\lambda_k)t} a(t)\mathrm{d}t}_{\text{Inverse Fourier transform of } a(t)} \right|^2 = \arg\max_\theta \underbrace{\sum_k p_k F(\theta-\lambda_k)}_{\text{Mixtures of Gaussians}}$$

$$F(x) \coloneqq \int a(t) e^{\mathbf{i}xt} \mathrm{d}t$$

$$a(t) \approx \exp\left(-\frac{x^2}{2T^2}\right) \longleftrightarrow F(x) \approx \exp\left(-\frac{T^2x^2}{2}\right)$$

A rough localization for the optimizer

$$\sum_k p_k F(\theta - \lambda_k) \approx \sum_k p_k \exp\left(-\frac{T^2}{2}(\theta - \lambda_k)^2\right)$$



$$|\theta^\star - \lambda_0| \leq \frac{C}{T_{\max}}$$

width $= \mathcal{O}\left(\frac{1}{T}\right) = \tilde{\mathcal{O}}\left(\frac{1}{T_{\max}}\right)$

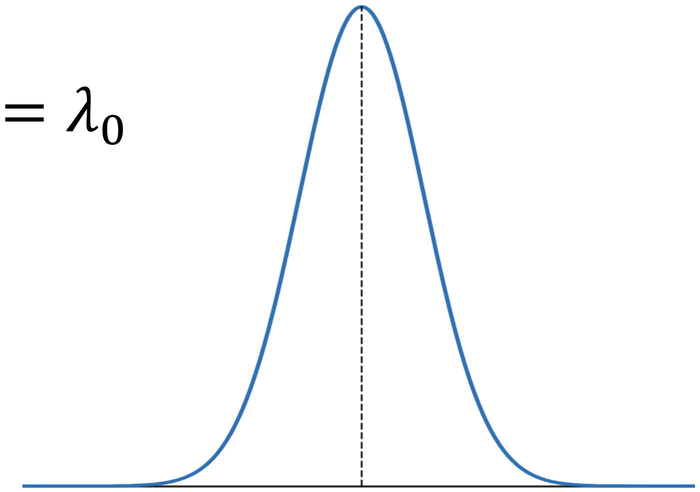
A finer error bound for the optimizer

$$p_0 \exp\left(-\frac{T^2}{2}(\theta-\lambda_0)^2\right) + \underbrace{\sum_{k>0} p_k \exp\left(-\frac{T^2}{2}(\theta-\lambda_k)^2\right)}_{\mathrm{Error}(\theta)}$$

$|\mathrm{Error}(\theta)| \leq 1 - p_0$

$p_0 = 1$:

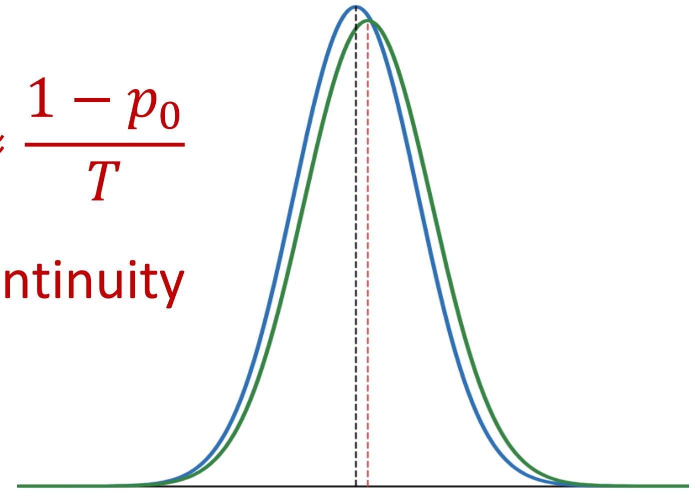
$\theta^\star = \lambda_0$



$p_0 \approx 1$:

$$|\theta^\star - \lambda_0| \approx \frac{1-p_0}{T}$$

By Lipschitz continuity



Quantum complex exponential least squares

Theorem (Ding-Lin ’23). Assume $p_0 > 0.5$. There exists an algorithm (QCELS) such that, with high probability, it outputs $\left|\hat{\lambda} - \lambda_0\right| \leq \epsilon$ with

- Maximal evolution time $T_{\max} = \mathcal{O}\left(\frac{1-p_0}{\epsilon}\right)$
- Total evolution time $T_{\text{total}} = \mathcal{O}\left(\frac{1}{\epsilon}\right)$

It is hard to directly prove the Heisenberg-limited scaling. In their paper, they use a multi-level strategy by choosing the Gaussian variance $\{T_j = 2^j T_0\}$ and shrinking the search domains of θ

Unified framework

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3 Classically post-process the dataset $\{(t_i, Z_i)\}_{i=1}^{N_S}$

QCELS:

A randomize grid sampled from a truncated Gaussian

- $T_{\mathrm{max}} = \mathcal{O}\left(\frac{1-p_0}{\epsilon}\right)$
- $T_{\mathrm{total}} = \mathcal{O}(\epsilon^{-1})$

$$\arg\min_{r,\theta} \frac{1}{N_S} \sum_{n=1}^{N_S} \left| Z_{t_n} - re^{-\mathbf{i}\theta t_n} \right|^2$$

Post-Kitaev phase estimation

1. Robust phase estimation
2. Optimization
3. Filtering
4. (Classical super-resolution methods)

The spectral density

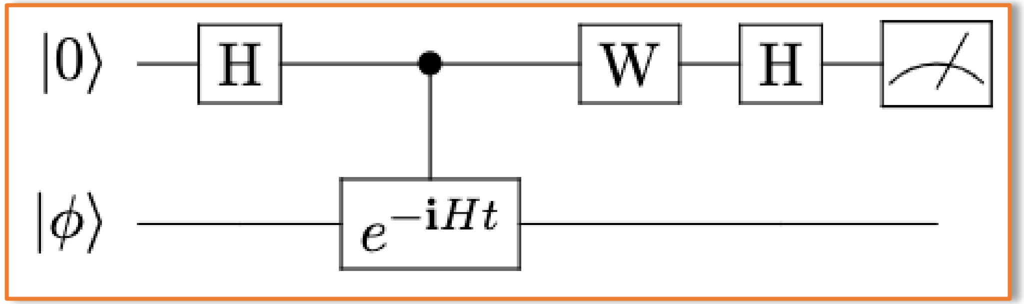
An initial guess $|\phi\rangle$ induces a probability distribution which we call the spectral density:

$$\mu(x) \coloneqq \sum_k p_k \delta(x - \lambda_k)\,,$$

where $p_k = |\langle\phi|E_k\rangle|^2$ and δ is the Dirac delta function

- $\sum_k p_k = 1$
- If $X \sim \mu$, then $\Pr[X = \lambda_k] = p_k$
- This distribution contains all the information about the spectrum

The spectral density



The Hadamard test circuit outputs the expectation value

$$\langle\phi|e^{-\mathbf{i}Ht}|\phi\rangle = \sum_k p_k e^{-\mathbf{i}\lambda_k t} = \int \mu(x) e^{-\mathbf{i}xt} \mathrm{d}x = \hat{\mu}(t)$$

- This is the Fourier transform of the spectral density $\mu(x)$
- For each t_n, $Z_n = \hat{\mu}(t_n) + e(t_n)$ with $\mathbb{E}[e(t_n)] = 0$

Filtering

Filtering by convolution:

$$(\mu \star F)(x) \xleftrightarrow{\text{FT/IFT}} \hat{\mu}(t)\hat{F}(t)$$

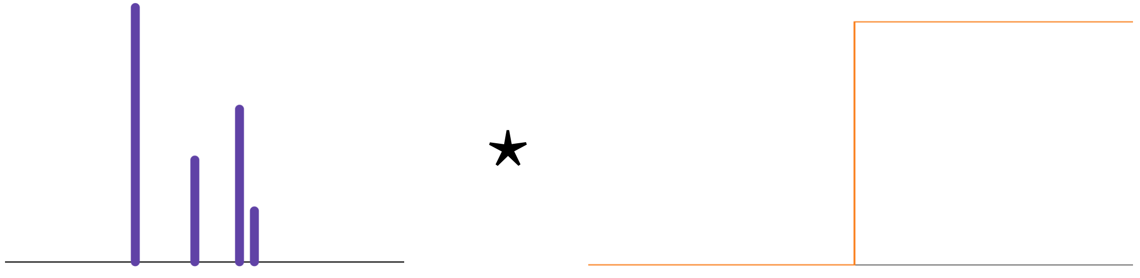
- Sample $t_n \sim \mu_F(t) \propto \left|\hat{F}(t)\right|$, and let Z_n be the sample from the Hadamard test

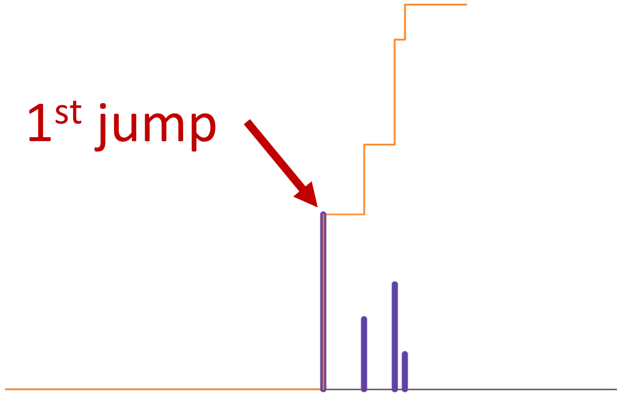
$$\mathbb{E}\left[Z_n e^{\mathbf{i}(\phi(t_n)+t_n x)}\right] = \int \hat{\mu}(t) e^{\mathbf{i}tx} e^{\mathbf{i}\phi(t_n)} \left|\hat{F}(t)\right| \mathrm{d}t = \int \hat{\mu}(t)\hat{F}(t) e^{\mathbf{i}tx} \mathrm{d}t = (\mu \star F)(x)$$

- We get an approximate evaluator for $\mu \star F$:

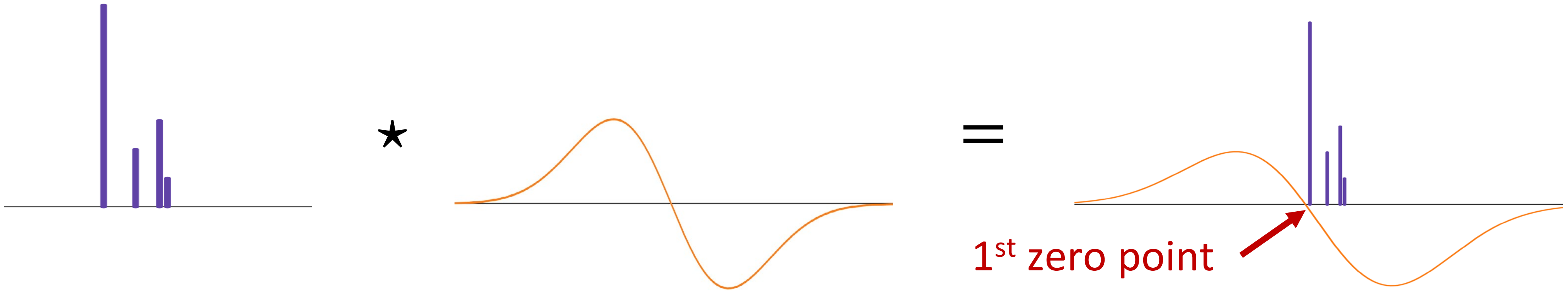
$$\frac{1}{N_S} \sum_{n=1}^{N_S} Z_n e^{\mathbf{i}(\phi(t_n)+t_n x)}$$

Filter 1: the Heaviside function (Lin-Tong ’22)

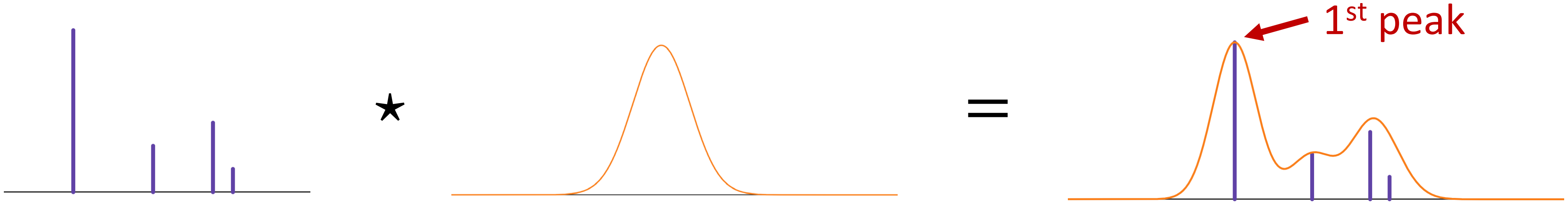




Filter 2: Gaussian derivative (Wang-França-**Z.**-Zhu-Johnson ’23)



Filter 3: Gaussian (Ding-Li-Lin-Ni-Ying-**Z.** ’24)



Quantum Multiple Eigenvalue Gaussian filtered Search

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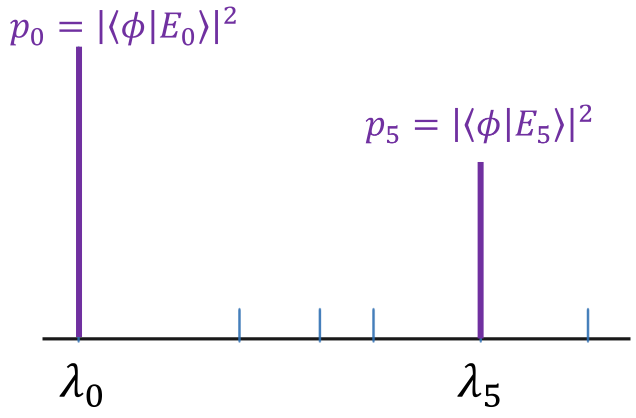
2 Run Hadamard tests with evolution times $\{t_i\}_{i=1}^{N_S}$

3 Classically post-process the dataset $\{(t_i, Z_i)\}_{i=1}^{N_S}$

QMEGS:

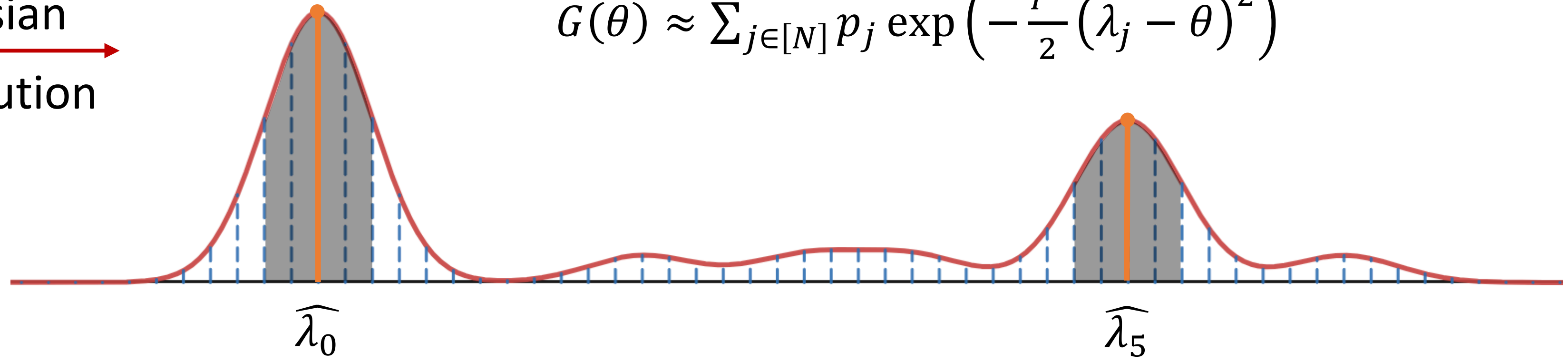
A randomize grid sampled from a truncated Gaussian



Gaussian convolution

"Mixture of Gaussians"

$$G(\theta) \approx \sum_{j\in[N]} p_j \exp\left(-\frac{T^2}{2}(\lambda_j - \theta)^2\right)$$



(Ding, Li, Lin, Ni, Ying, **Z.**, Quantum 2024)

The strongest theoretical guarantees by QMEGS

- Dominant eigenvalues: $\{\lambda_k\}_{k\in\mathcal{D}}$ with $p_{\min} \coloneqq \min_{k\in\mathcal{D}} p_k$
- Tail eigenvalues: $\{\lambda_k\}_{k\in\mathcal{D}^c}$ with $p_{\text{tail}} \coloneqq \sum_{j\in\mathcal{D}^c} p_j$
- Sufficient Overlap Assumption:

$$p_{\text{tail}} \ll p_{\min}$$

- No gap: $T_{\text{total}} = \text{poly}(\epsilon^{-1})$ even some eigenvalues are very close to each other
- "Short" depth: $T_{\max} = \tilde{\mathcal{O}}(p_{\text{tail}}\epsilon^{-1})$

Algorithms	Properties			
	Allow $p_{\text{tail}} > 0$	Heisenberg limit	No gap requirement	"Short" depth
QEEA [Som19]	✓	✗	?	✗
ESPRIT [SHT22]	?	✗	?	✗
[DTO22]	?	✓	✓	✗
[LNY23a, Theorem III.5]	✓	✓	✓	✗
[LNY23a, Theorem V.1]	✓	✓	✗	✓
MM-QCELS [DL23b]	✓	✓	✗	✓
QMEGS (this work)	✓	✓	✓	✓

(Ding, Li, Lin, Ni, Ying, **Z.**, Quantum 2024)

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1. Robust phase estimation
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ESPRIT:

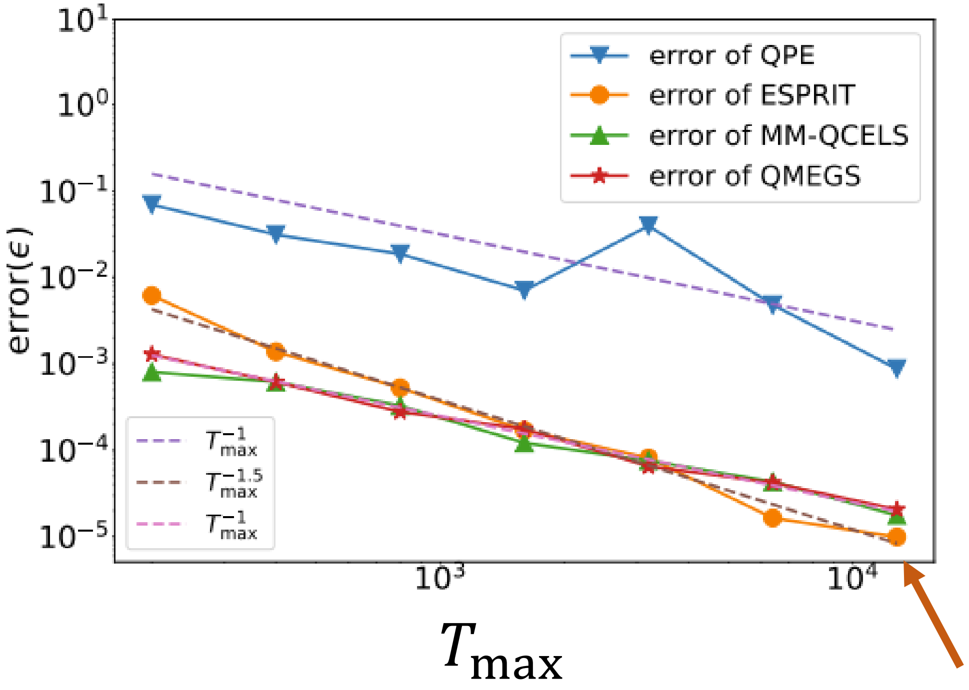
A uniform grid $t_i = i$

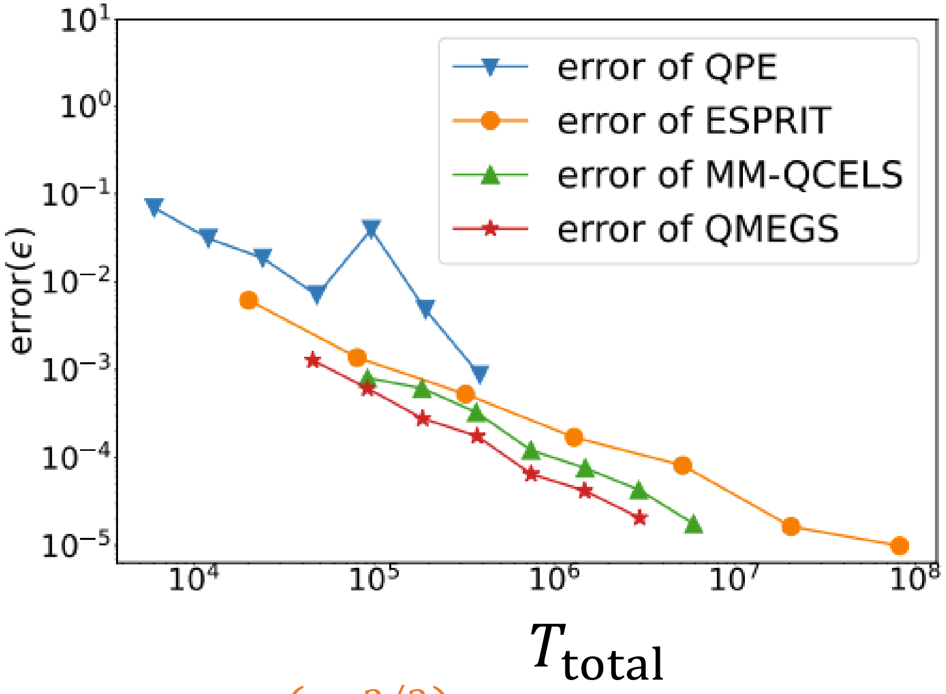
- $T_{\max} = \mathcal{O}\left(\epsilon^{-2/3}\right)$
- $T_{\text{total}} = \mathcal{O}\left(\epsilon^{-4/3}\right)$
  (no Heisenberg-limited scaling)

Run ESPRIT algorithm

Numerical simulation and resource estimation

1d TFIM Hamiltonian





ESPRIT achieves $T_{\max} = \mathcal{O}\left(\epsilon^{-2/3}\right)$

More extensions

- Computing ground state (or eigenstate) observable expectation values $\langle E_0|O|E_0\rangle$ using a modified circuit (**Z.**-Wang-Johnson ’21; Zeng-Sun-Yuan ’21, Sun et al. ’24…)
- Approximate Hamiltonian simulation using Trotter and randomized compiling (Wan-Berta-Campbell ’21)
- Robustness under simple noise models (Kshirsagar-Katabarwa-Johnson ’22; Ding-Dong-Tong-Lin ’22)
- Zero-ancilla phase estimation (Yang et al. ’24)
- Estimating ground state degeneracy or density of states (Ding-Lin-Yang-**Z.** ’25)