Even Shorter Quantum Circuit for Phase Estimation on Early Fault-Tolerant Quantum Computers

Ibrahim Abdulazeez

2024

Problem: Quantum Phase Estimation.

Method: Quantum Complex Exponential Least Squares (QCELS).

Device: (Constraint) Early Fault-Tolerant Quantum Computer.

Introduction:

- Main problem, input, complexity.

Quantum Circuit and Data Generation Process

- Data Set Preparation and Post-processing

Method: QCELS

- Solve the optimization problem, Heuristic theorem, Intuitive analysis.

Theorem for large $\mathbf{p}_0$

Multi QCELS

Algorithm for small $\mathbf{p}_0$

Conclusion

Main Problem

Given a Hamiltonian $H \in \mathbb{C}^{d \times d}$, $d \gg 1$, we estimate the smallest eigenvalue λ_0 (Ground state energy).

Assume: $\lambda_0 \in [-\pi, \pi)$

corresponding eigenvector of $|\psi_0\rangle \in \mathbb{C}^d$

Input:

The problem is QMA-hard.

Common additional assumption: good initial state

$$|\psi\rangle = U_I|0^n\rangle$$

.

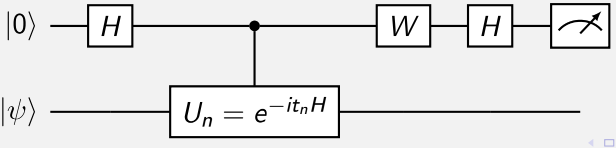
- Initial State:

$$|\psi\rangle \in \mathbb{C}^d$$

$$0 < p_0 = |\langle\psi|\psi_0\rangle|^2 < 1$$

- Quantum Oracle: Given any

$$t_n \in R$$



Quantum Circuit and Hadamard Test

To achieve this, our quantum circuit above is the same as the circuit used in the Hadamard test but replaces $U = e^{-i\tau H}$ by $U_n = e^{-in\tau H}$ for a sequence of integers n.

This simple circuit:

- Uses only one ancilla qubit.
- Is suitable for early fault-tolerant quantum computers.

Quantum Circuit Details

Definitions:

- τ is the time step used in the controlled time evolution.
- $t_n = n\tau$, where $n = 0, \ldots, N-1$, defines the discrete time steps.
- Z_n is a complex-valued random variable such that $E(Z_n) = \langle\psi|e^{-it_nH}|\psi\rangle$.

Circuit Operation:

The circuit provides an estimate of $\langle\psi|e^{-it_nH}|\psi\rangle$ by measuring the success probability of the first qubit.

Repeated measurements at different n provide a complex time series:

$$\{(t_n, Z_n)\}_{n=0}^{N-1}$$

where Z_n approximates $\langle\psi|e^{-it_nH}|\psi\rangle$.

Complexity

$$\{t_n\}_{n=1}^{N} \in \mathbb{R} \longrightarrow \dots$$

Maximum Running Time:

$$T_{\text{max}} = (N-1)\tau \textbf{ for simplicity } T_{max} = N\tau$$

How large does our quantum computer need to be?

Total Running Time:

$$T_{\text{total}} = \sum_{n=1}^{N} |t_n|$$

How long will we need to run it?

Complexity

Classical Result: To ensure $|\lambda - \lambda_0| \leq \epsilon$:

$$\text{When } P_0 = 1, \quad T_{\max} = O(1), \quad T_{\text{total}} = O\left(\frac{1}{\epsilon^2}\right)$$

(Hadamard Test).

$$\text{Any} \quad P_0, \quad T_{\max} > \frac{\pi}{\epsilon}, \quad T_{\text{total}} = O\left(\frac{1}{\epsilon}\right)$$

(Heisenberg-limited QPE).

Goal: For any P_0,

$$T_{\max} > \frac{\pi}{\epsilon} \quad \text{(Reduce)}, \quad \text{such that} \quad T_{\text{total}} = O\left(\frac{1}{\epsilon}\right) \quad \text{(QPE)}.$$

Complexity

Our Method, for $P_0 \geq 0.71$,

$$T_{\text{max}} \leq \frac{\pi}{\epsilon}, \quad T_{\text{total}} = O\left(\frac{1}{\epsilon}\right)$$

Any P_0,

$$T_{\text{max}} > \frac{\pi}{\epsilon}, \quad T_{\text{total}} = O\left(\frac{1}{\epsilon}\right) \quad \text{(QPE).}$$

Informal Theory

$$T_{\max} = O\left(\frac{\sqrt{1-p_0}}{\epsilon}\right)$$

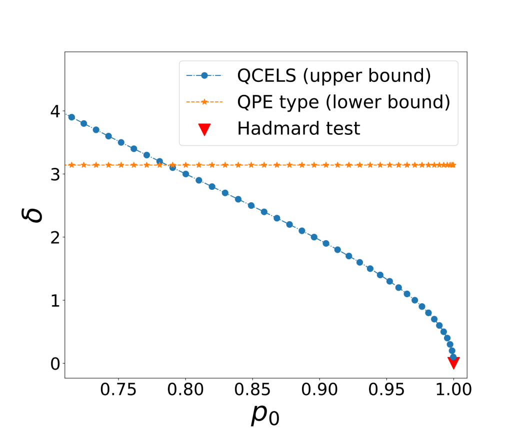


Figure: Depth theory

Quantum Circuit and Data Generation Process

- **Quantum Circuit:** Fig. 1 shows a quantum circuit designed to generate data points for the Hamiltonian H.
- **Random Variables:**
  - Set $W = I$, measure ancilla qubit:

$$X_n = \begin{cases} 1 & \text{if outcome is } 0 \\ -1 & \text{if outcome is } 1 \end{cases}$$

$$E(X_n) = \mathrm{Re}\langle\psi|\exp(-in\tau H)|\psi\rangle$$

  - Set $W = S^\dagger$, measure ancilla qubit:

$$Y_n = \begin{cases} 1 & \text{if outcome is } 0 \\ -1 & \text{if outcome is } 1 \end{cases}$$

$$E(Y_n) = \mathrm{Im}\langle\psi|\exp(-in\tau H)|\psi\rangle$$

Data Set Preparation and Postprocessing

- **Input Parameters:** Given two preset parameters $N, N_s > 0$ and time step $\tau > 0$, the data set is generated.
- **Data Set D_H:**

$$D_H = \{(n\tau, Z_n)\}_{n=0}^{N-1}$$

By running the quantum circuit N_s times Z_n is calculated as:

$$Z_n = \frac{1}{N_s} \sum_{k=1}^{N_s} (X_{k,n} + iY_{k,n})$$

- **Key Result:** In the limit $N_s \to \infty$,

$$Z_n = \langle \psi | \exp(-in\tau H) | \psi \rangle$$

- **Simulation Time:**
  - Maximal simulation time: $T_{\max} = (N-1)\tau$
  - Total simulation time: $\frac{N N_s T_{\max}}{2}$

Quantum Complex Exponential Least Squares

- Time t
- Sampled real and imaginary parts over time

Objective:

$$(r^*, \theta^*) = \arg \min_{r\in\mathbb{C}, \theta\in\mathbb{R}} L(r, \theta)$$

where the loss function is defined as:

$$L(r, \theta) = \frac{1}{N} \sum_{n=0}^{N-1} \left| Z_n - re^{-it_n\theta} \right|^2$$

Output: θ^* is the estimate for the phase λ_0.

Note: Fitting may not be exact if $p_0 < 1$, but it can still estimate λ_0 accurately.

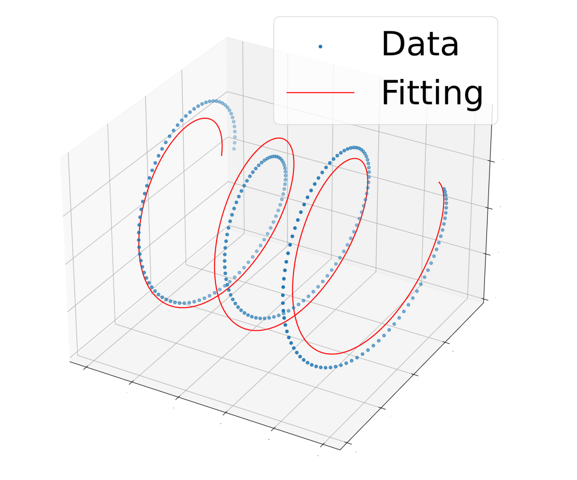


Figure: Data fitting

Solve the Optimization Problem

Step 1: Fix θ, optimize r:

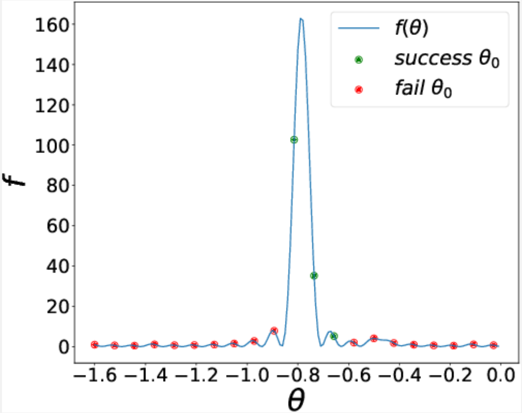
$$\min_{r\in\mathbb{C}} L(r,\theta) = \frac{1}{N}\sum_{n=0}^{N-1}|Z_n|^2 - \frac{1}{N}\left|\sum_{n=0}^{N-1} Z_n e^{i\theta n\tau}\right|^2$$

Step 2: Optimize with respect to θ:

$$\theta^* = \arg\max_{\theta\in\mathbb{R}} f(\theta), \quad f(\theta) = \frac{1}{N}\left|\sum_{n=0}^{N-1} Z_n e^{i\theta n\tau}\right|^2$$

Energy Landscape: The landscape is rugged but can be handled classically since θ is a scalar.

Optimization Landscape



Informal Theory

$$T_{\max} = O\left(\frac{\sqrt{1-p_0}}{\epsilon}\right)$$

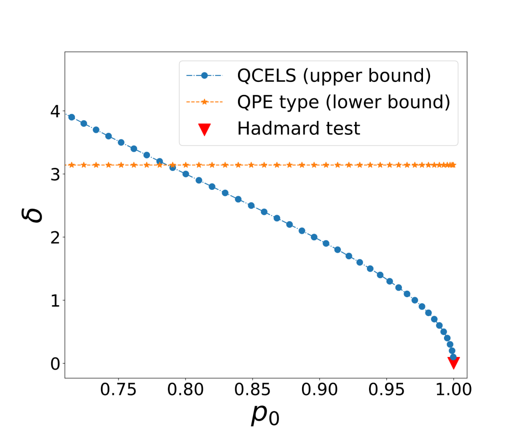


Figure: Depth theory

Heuristic Theorem: Maximal Run Time

Heuristic Theorem (General Result) for large $\mathbf{P}_0$:

Assume the overlap p_0 between the initial state and the target eigenstate is very large. In this case,

$$\delta = \Theta(\sqrt{1 - p_0}), \quad T_{\mathbf{max}} = \frac{\delta}{\epsilon}$$

Let θ^* be the optimizer:

$$|(\theta^* - \lambda_0) \mod [-\pi/\tau, \pi/\tau]| < \epsilon.$$

Key Result:

$$T_{\mathbf{max}} = O\left(\frac{\delta}{\epsilon}\right)$$

where $\delta \sim \sqrt{1 - p_0}$. This holds for sufficiently large p_0.

Intuitive Analysis of Basic Version of QCELS

Recall:

$$\theta^* = \arg\max_{\theta \in \mathbb{R}} f(\theta), \quad f(\theta) = \frac{1}{N} \left| \sum_{n=0}^{N-1} Z_n e^{i\theta n\tau} \right|^2 .$$

Objective: Bound

$$R_0 = |(\lambda_0 - \theta^*)\tau \mod [-\pi, \pi]|.$$

Lower bound on $f(\lambda_0)$:

$$(2p_0 - 1)N \leq \sqrt{f(\lambda_0)}.$$

Upper bound on $f(\theta^*)$:

$$\sqrt{f(\theta^*)} \leq \left| \frac{\sin(NR_0/2)}{\sin(R_0/2)} \right| + (1 - p_0)N.$$

Intuitive Analysis of Basic Version of QCELS

Optimality Condition:

$$\sqrt{f(\theta^*)} \geq \sqrt{f(\lambda_0)} \quad \Rightarrow \quad \left|\frac{\sin(NR_0/2)}{\sin(R_0/2)}\right| \geq (3p_0 - 2)N.$$

Approximation:

$$\frac{\sin(N(\delta/2N))}{\sin(\delta/2N)} \approx N\left(1 - \frac{\delta^2}{24}\right).$$

$$\delta^2 \approx 72(1 - p_0) \quad \Rightarrow \quad \delta \to 0 \text{ as } p_0 \to 1.$$

Since $\frac{\sin(Nx)}{\sin(x)}$ is decreasing on $[0, \pi/(2N)]$, we conclude:

$$R_0 \leq \frac{\delta}{N} \quad \text{or} \quad |(\lambda_0 - \theta^*) \mod [-\pi/\tau, \pi/\tau]| < \frac{\delta}{T_{\max}} = \epsilon.$$

This gives $T_{\max} = \frac{\delta}{\epsilon}$: short runtime!

Theorem for Large but specific p_0

Theorem 1:
If $p_0 > 0.71$, choose

$$\delta = \Theta\left(\sqrt{1-p_0}\right).$$

There exists an algorithm that uses 1 ancilla qubit to estimate λ_0 to precision ϵ with:

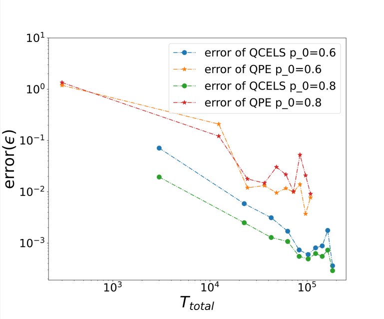
$$T_{\max} = \frac{\delta}{\epsilon}, \quad T_{\text{total}} = \tilde{\Theta}\left(\delta^{-(1+o(1))}\epsilon^{-1}\right).$$

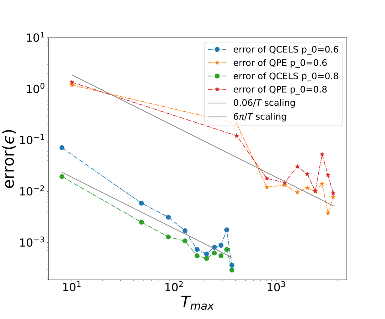
Distinct Feature:

- The preconstant δ can be arbitrarily small as $p_0 \to 1$.

Numerical evidence

Transverse Field Ising Model (TFIM).





- Numerical performance is much better than theoretical prediction, and the bound 0.71 can be pushed downward.
- Two order of magnitude reduction of maximal runtime!

Convergence - Basic Version of QCELS

Theorem (Basic version of QCELS):
Given $p_0 > 0.71$, we can choose:

$$\delta = \Theta(\sqrt{1 - p_0}), \quad T_{\text{max}} = \frac{\delta}{\epsilon}, \quad NN_s = \Omega(\delta^{-(2+o(1))})$$

Let θ^* be the optimizer. Then with high probability:

$$|(\theta^* - \lambda_0) \mod [-\pi/\tau, \pi/\tau]| < \epsilon.$$

Key Results:

- Short maximal runtime (circuit depth).
- Does not achieve Heisenberg-limited scaling.

Scalings:

$$T_{\text{max}} = N\tau \quad \Rightarrow \quad N = O(\epsilon^{-1}) \text{ if } \tau \text{ is small.}$$

$$T_{\text{total}} = \tau N_s N(N-1)/2 = O(\epsilon^{-2}).$$

Multi-level QCELS

Multi-level QCELS:
The result $T_{\max} = \frac{\delta}{\epsilon}, NN_s = \Omega(\delta^{-(2+o(1))})$ is independent of τ.

$$|(\theta^* - \lambda_0) \mod [-\pi/\tau, \pi/\tau]| < \epsilon.$$

Algorithm: For $j = 1, \ldots, J$:

1. Generate data set $D_{H,j} = \{(n\tau_j, Z_{n,j})\}_{n=0}^{N-1}$.
2. Solve $(r_j^*, \theta_j^*) = \arg\min_{r \in \mathbb{C}, \theta \in [-\lambda_{\min}, \lambda_{\max}]} L(r, \theta)$.
3. Shrink search interval:

$$\lambda_{\min} = \theta_j^* - \frac{\pi}{2\tau_j}, \quad \lambda_{\max} = \theta_j^* + \frac{\pi}{2\tau_j}.$$

Convergence - Multi-level QCELS

Theorem (Multi-level QCELS):
If $p_0 > 0.71$, choose:

$$\delta = \Theta(\sqrt{1-p_0}), \quad T_{\max} = \frac{\delta}{\epsilon}, \quad T_{\text{total}} = \Theta\left(\delta^{-(1+o(1))}\epsilon^{-1}\right).$$

Let θ^* be the output of multi-level QCELS. Then with high probability:

$$|(\theta^* - \lambda_0) \mod [-\pi, \pi]| < \epsilon.$$

Key Results:

- Short maximal runtime (circuit depth).
- Achieves Heisenberg-limited scaling.

Algorithm for Small p_0

Proposed Algorithm:

- Combines the multilevel QCELS algorithm with the Fourier-filtering technique from Ref. [15] to estimate λ_0.

Relative Overlap $p_r(I, I')$:

$$p_r(I, I') = \frac{|\langle\psi|\psi_0\rangle|^2 1_I(\lambda_0)}{\sum_{\lambda_k \in I'} |\langle\psi|\psi_k\rangle|^2},$$

where $1_I(\cdot)$ is the indicator function on I, and $\lambda_0 \in I$.

Scenario with Spectral Gap $\Delta = \lambda_1 - \lambda_0$:

- Choose intervals $I = [-\pi, \lambda_{\text{prior}} + \Delta/4]$ and $I' = [-\pi, \lambda_{\text{prior}} + 3\Delta/4]$.
- The distance between I and $(I')^c$ is $D = \Delta/2$.
- Relative overlap $p_r(I, I')$ is 1 when $|\lambda_{\text{prior}} - \lambda_0| \leq \Delta/4$.

Note: Even with a small spectral gap, appropriate intervals I and I' can result in a larger distance D and still achieve a large relative overlap.

Small p_0

Theorem

Given relative overlap $p_r(I, I') \geq 0.71$ and $D = \min_{x_1 \notin I', x_2 \in I} |x_1 - x_2|$, choose

$$\delta = \Theta\left(\sqrt{1 - p_r(I, I')}\right).$$

There exists an algorithm that uses 1 ancilla qubit to estimate λ_0 to precision ϵ with:

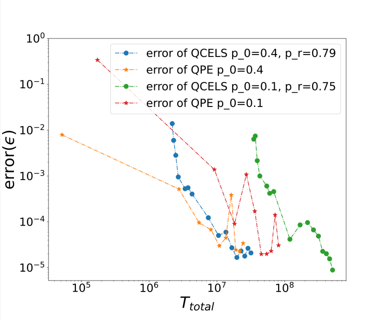
$$T_{\max} = \tilde{\Theta}(D^{-1}) + \frac{\delta}{\epsilon}, \quad T_{\text{total}} = \tilde{\Theta}\left(p_0^{-2}\delta^{-(2+o(1))}(D^{-1} + \frac{\delta}{\epsilon})\right).$$

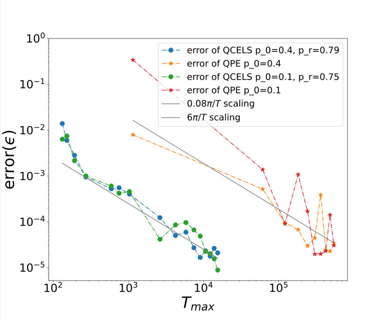
Distinct Features:

- Uses information of relative overlap (previous algorithms are agnostic to this).
- Reduces circuit depth when $D \ll \epsilon$ and $p_r(I, I')$ is large.

Numerical evidence

Hubbard.





- Two order of magnitude reduction of maximal runtime!

Conclusion

Conclusion:

- QCELS is efficient for estimating the ground state energy on early quantum computers.
- It reduces the maximal and total runtime significantly, making it a powerful method for quantum phase estimation.

Thank you!