Benchmarking Quantum Phase Estimation with Physical Hamiltonians

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Abstract

We studied three different quantum phase estimation (QPE) algorithms, the standard QPE, iterative QPE and Bayesian iterative QPE. We then used three unique physical systems, the quantum harmonic oscillator, H_2 molecule and the Ising model in order to benchmark the accuracy and resource efficiency of the algorithms.

1 Introduction

As part of MIT's iQuHack event, we were tasked with creating a project that utilized Quantinuum's Nexus platform to explore different variants of the quantum phase estimation algorithm. We instantiated these algorithms using TKET and then utilized Hamiltonians of solved physical systems as a testing ground for benchmarking and comparing the utility of our phase estimation algorithms. The emulator provided by the Nexus platform implements a noise model based on the noise found on the H-Series quantum computers. This allows us to effectively benchmark each algorithm with realistic error rates based on depth and complexity of gates in a given circuit.

2 Variants of Quantum Phase Estimation

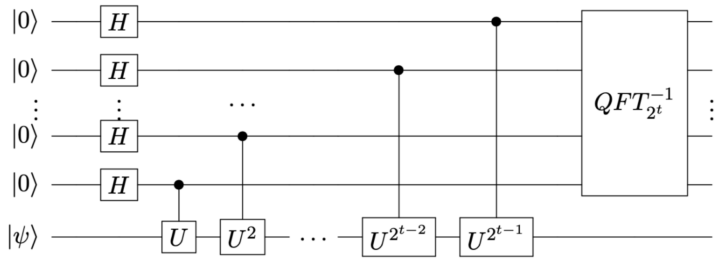
2.1 Standard Quantum Phase Estimation

Given some unitary time evolution operator U and eigenvector $|\psi\rangle$ of U, the goal of the phase estimation algorithm is to estimate θ where

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

The circuit is constructed with p input qubits that make up the state vector $|\psi\rangle$ and t measurement qubits that are used to approximate θ. The critical block that allows Quantum Phase Estimation (QPE) to be realized is the inverse quantum Fourier transform ($QFT^\dagger$).

$$QFT^\dagger : \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi ijk/N}|k\rangle \longmapsto |j\rangle , \quad N = 2^n$$

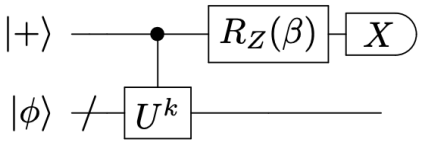


Initially, Hadamard gates are applied on the measurement register so that the resulting state is a uniform superposition across all possible states. Then, a controlled-U gate, which is related to a given system's Hamiltonian by $U = e^{\frac{-iHt}{\hbar}}$ is applied to the measurement qubits. Each additional measurement qubit has twice the applications of U as the previous measurement qubit. The inverse quantum Fourier transform is then applied to the measurement register. A measurement on these qubits then returns an t-bit approximation of θ of the form $0.\theta_1\theta_2\ldots\theta_t$ where $\forall i \in [t] : \theta_i \in \{0, 1\}$ and

$$\theta = \frac{\theta_1}{2} + \frac{\theta_2}{2^2} + ... + \frac{\theta_t}{2^m}$$

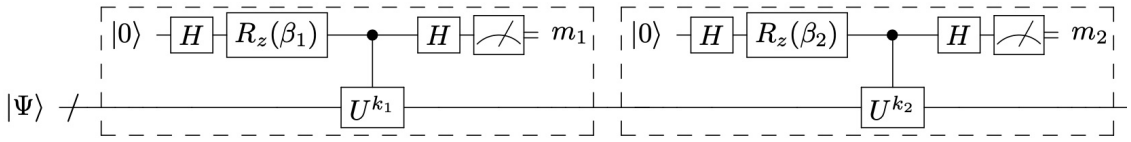
While this textbook QPE implementation works in theory, the depth and complexity of the circuit leads to high error rates when run on a noisy quantum computer. In order to implement phase estimation, accounting for the noise in a quantum computer, algorithms with smaller circuit depths and the use of Bayesian statistics have been proposed.

2.2 Iterative Quantum Phase Estimation



Iterative Quantum Phase Estimation (IQPE)[1] utilizes a single measurement qubit rather than t measurement qubits. However, to estimate the phase to t bits of precision, it runs t different circuits over the course of t rounds rather than running a single quantum circuit, where the circuits in each round may depend on the results of previous rounds. Notably, IQPE does not require the use of an inverse QFT block. The breaking of the quantum phase estimation into rounds is advantageous for noisy-intermediate scale quantum computers, since iterative quantum phase estimation requires smaller circuit depths than standard QPE, resulting in less noise. In the k-th round, IQPE runs a controlled U^{2^m-k} unitary and then applies a Z rotation of $\beta = -2\pi(\sum_{j=0}^{k} \frac{\theta_{m-j}}{2^{k-j+2}})$, where θ_m is the least significant bit and θ_1 is the most significant bit of the phase being estimated. The bits are received in reverse order, from θ_m to θ_1.

2.3 Bayesian Quantum Phase Estimation



Bayesian Quantum Phase Estimation (BQPE)[2][3] builds upon the idea of IQPE by more efficiently conducting its phase shift component β_r where $r \in R$ represents a specific round. The advantage stems from each rounds ability to be parameterized by its k^r and β_r factor. By reading out the measurements m we can update the prior set and express the posterior distribution resulting as:

$$P^{(r+1)}(\phi, w) = \frac{P_{k,\beta}(m|\phi, w) \cdot P^r(w, \phi)}{\phi^r_{k,\beta}(m)}$$

This equation essentially takes the most recently measured result and re-inputs it into the circuit as the now posterior state so the circuit is continuous updated with a better idea of how much to rotate about the Z-axis. From the above equation β can be calculated if the k^r value is known by utilizing the previous coefficients. Because of this continuous updating BQPE has particular advantage in noisy systems. The noise can be accounted for by modeling noise in a particular system. For example, depolarizing noise provides noise free measurement with probability p and uniformly random measurement with $1-p$. If this type of noise was present then modify the $P_{k,\beta}(m|\phi_j)$ term in the above equation to equal $p \cdot |_{k,\beta}(m|\phi_j) + \frac{1-p}{2}$. Now when recalculating β, each iteration can better account for this margin of error and correct accordingly.

3 Benchmarking on Physical Models

3.1 Harmonic Oscillator

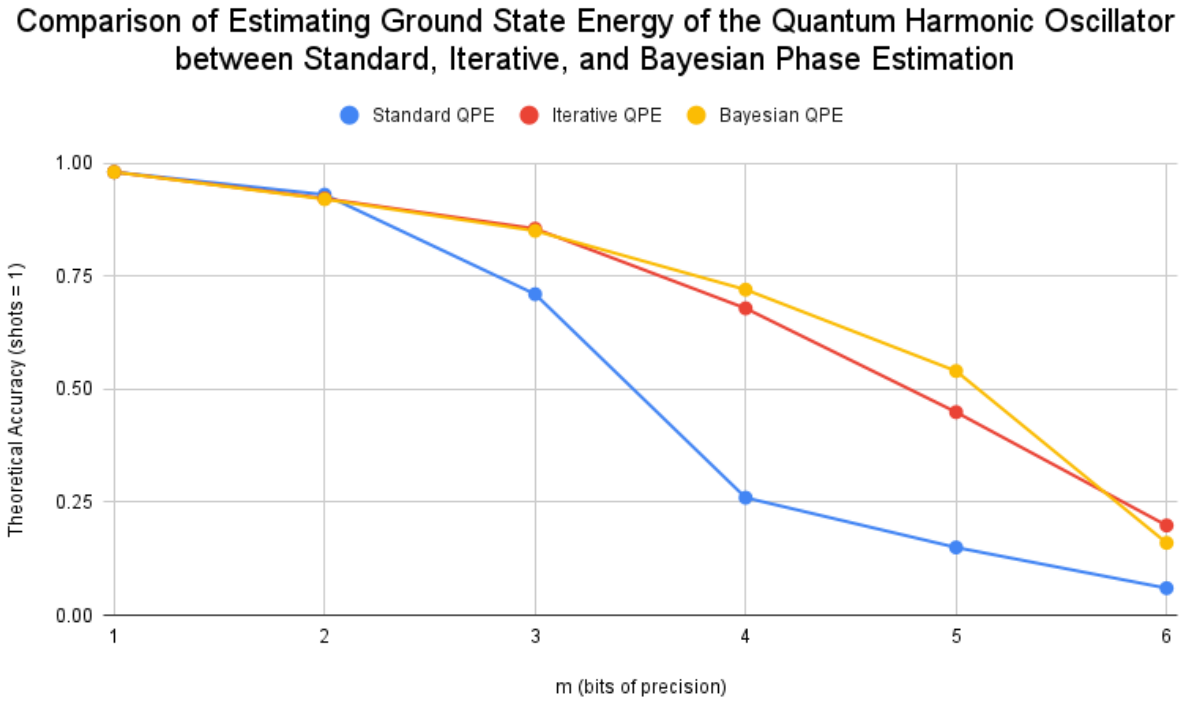


Figure 1: We ran tasks of increasing complexity on the Quantinuum H1-E emulator in a head-to-head comparison between standard, iterative, and Bayesian quantum phase estimation (QPE). We attempted to estimate the ground state energy of a quantum harmonic oscillator, varying the digits of precision allowed (thereby increasing the number of gates used), and found an estimate for the theoretical accuracy each phase estimation algorithm would have for correctly estimating the eigenvalue to the desired precision given a single shot. Standard QPE has an accuracy that decays more rapidly than Iterative QPE's due to the effects of greater depth circuits, while Bayesian QPE performed similarly in terms of theoretical accuracy to Iterative QPE. However, Bayesian QPE required significantly fewer total gates than Iterative QPE (See Figure 2)

The Harmonic Oscillator is one of the simplest yet most effective theoretical models used to analyze many physical systems. In the 1D case the Hamiltonian is given by

$$H\left|\psi\right\rangle = (-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + mw^2\hat{x}^2)\left|\psi\right\rangle = E\left|\psi\right\rangle$$

Solutions to this differential equation can be used to find eigenvalues that correspond to the energy levels of the system. These energies are given by

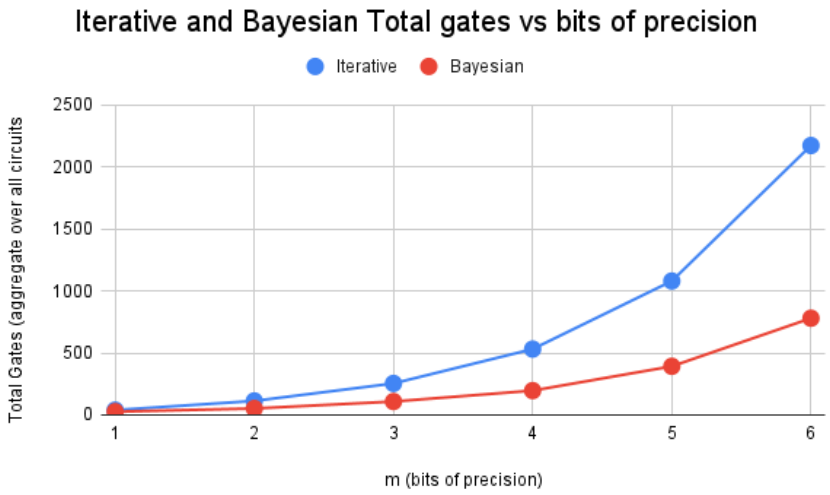


Figure 2: Scaling of number of gates (in aggregate over all compiled circuits run) vs. the bits of precision requested.

$$E_n = \hbar\omega(n + \frac{1}{2})$$

The solutions form an orthonormal basis so we can diagonalize this Hamiltonian with the corresponding energy eigenstates along the diagonal.

$$H = \begin{bmatrix} \frac{\hbar\omega}{2} & 0 & \dots & 0 \\ 0 & \frac{3\hbar\omega}{2} & \dots & 0 \\ \vdots & \vdots & \ddots & \\ 0 & 0 & & \hbar\omega(n+\frac{1}{2}) \end{bmatrix}$$

Because the Hamiltonian is diagonal it has the nice property that the time evolution operator U is also diagonal.

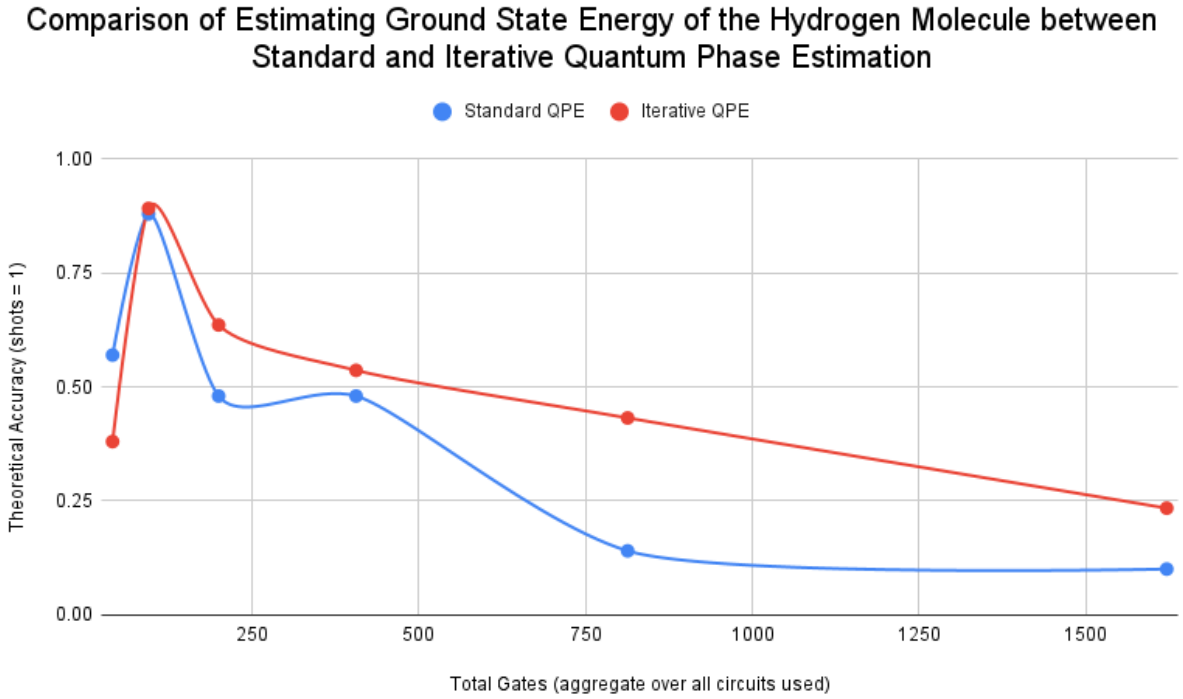
$$U = e^{\frac{-iHt}{\hbar}} = \begin{bmatrix} e^{\frac{-i\hbar\omega t}{2}} & 0 & \dots & 0 \\ 0 & e^{\frac{-3i\hbar\omega t}{2}} & \dots & 0 \\ \vdots & \vdots & \ddots & \\ 0 & 0 & & e^{-i\hbar\omega(n+\frac{1}{2})t} \end{bmatrix}$$

We then shift the energies down an amount $\frac{\hbar\omega}{2}$ so that the ground state energy is 0. With this U, we can then benchmark each QPE algorithms.

3.2 H_2 molecule

The effective Hamiltonian for the diatomic molecule H_2 is

$$H = h_1 Z_1 + h_2 Z_2 + h_3 Y_1 Y_2 + h_4 Z_1 Z_2 + h_5 I.$$



where $\{X_i, Y_i, Z_i\}$ are the Pauli X, Y, and Z operators acting on the i-th qubit, with $h_1, \ldots, h_5$ being some real coefficients (see [3] for full details). We follow the Hamiltonian for the molecular hydrogen used by [3] which was found using the Jordan-Wigner transformation. This model is more challenging than the quantum harmonic oscillator because, unlike in that Hamiltonian, there are off-diagonal terms in this Hamiltonian. Therefore the time evolution operator also has off-diagonal terms and we must solve for the eigenvectors to find the ground state. We used Mathematica to find exact eigenvectors and eigenvalues to benchmark our performance.

3.3 The Ising Model

The Ising Model Hamiltonian is

$$H = -\sum_{<i,j>} J_{ij} Z_i Z_j - \sum_i g_i X_i$$

Where J_{ij} scales the interaction between neighboring dipoles and g_i scales the global transverse field interaction in comparison to neighbor interactions.

When $J < 0$ the phase exhibits antiferromagnetic ordering while when $J > 0$ the phase exhibits ferromagnetic ordering. When $g = 0$ and $J > 0$ the ground state is 2-fold degenerate and has ground states $|00...00\rangle$ and $|11...11\rangle$

We have three qubits which can model a 1D, three dipole triangular lattice Ising model. While this is admittedly a rather boring Ising Model, it allows us to work with a unitary

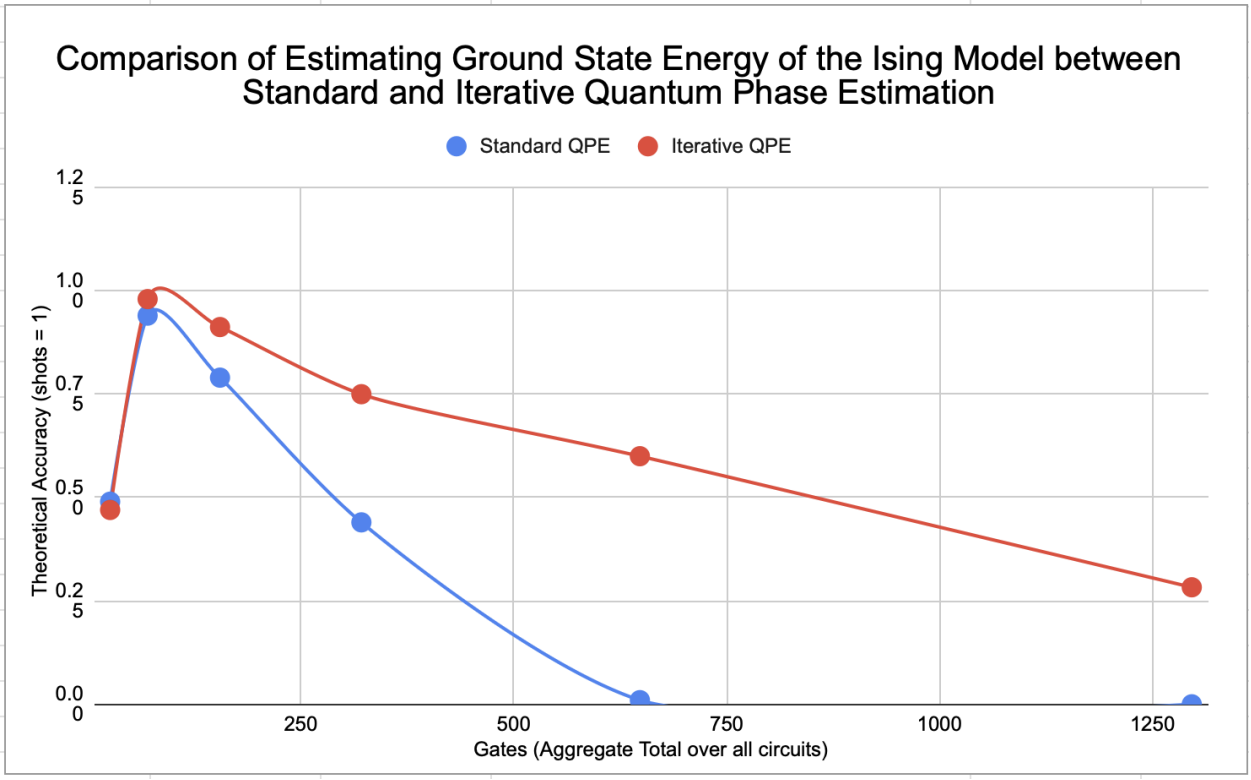


Figure 3: Comparison of Theoretical Accuracy of Standard and Iterative QPE as a function of total gates.

with off diagonal elements which we have solved entirely and therefore works as a good benchmark.

4 Conclusions

After benchmarking the algorithms on different physical Hamiltonians, we have found that the iterative QPE performs significantly better than the standard QPE when the machine has noise comparable to Quantinuum's H-Series quantum computers. The Bayesian QPE has inconclusive results, but performed slightly better on the quantum harmonic oscillator benchmark. The Bayesian's reliance on a continuously updating beta coefficient means it must constantly run classical algorithms in conjunction with its quantum one. Every iteration of the Bayesian, much like the Iterative PEA, has to calculate a new probability to achieve a better approximation. The difference is the Iterative PEA can be calculated on the quantum circuit while the Bayesian PEA must run a fast Fourier coefficient generator or a Von Mises coefficient approximation. Both of these represent substantial overhead. The benefit though is the beta calculations can be designed machine specifically to greatly reduce the impact of noise. This idea was stated previously with the depolarizing noise example. However as quantum computers improve and noise is corrected more efficiently this overhead may present problems than benefits.

References

[1] A. Kitaev, A. Shen, and Mikhail Vyalyi. "Classical and Quantum Computation". In: *The American Mathematical Monthly* 110 (Dec. 2003). DOI: 10.2307/3647986.

[2] Nathan Wiebe and Chris Granade. "Efficient Bayesian Phase Estimation". In: *Physical Review Letters* 117.1 (June 2016). ISSN: 1079-7114. DOI: 10.1103/physrevlett.117.010503. URL: http://dx.doi.org/10.1103/PhysRevLett.117.010503.

[3] Kentaro Yamamoto et al. *Demonstrating Bayesian Quantum Phase Estimation with Quantum Error Detection*. 2023. arXiv: 2306.16608 [quant-ph].