On the Phase Estimation Amplitudes in the Quantum Matrix Equation Solver

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Abstract—The phase estimation amplitude in the quantum matrix equation solver, namely the Harrow/Hassidim/Lloyd (HHL) algorithm is studied in this work. It is the periodic behavior of the amplitude with respect to the eigenvalue estimation error indicates the choice of the simulation time. The impact of the initial states on the quantum phase estimation (QPE) is also provided. This work is expected to be instructive for the formulation of the error analysis in HHL variants.

Index Terms—HHL, QPE, error analysis

I. Introduction

Electromagnetic simulation tools are vastly used to aid the design and assess the performance of high-speed interconnects [1]. Due to escalating design complexity, simulations become increasingly lengthy. An essential determinant of the simulation time is solving the matrix equation for the electromagnetic field. To accelerate the matrix equation solver, a plethora of work on fast algorithms [2] have been proposed for different formulations. Besides these classical methods, quantum algorithms have drawn the attention of researchers in the computational electromagnetic community [3], [4], mainly because the quantum matrix equation solver [5] can provide exponential speedup with respect to problem size compared to their classical counterparts. In the HHL algorithm, QPE is the crucial component dictating the error of the final state. In this paper, we study the QPE amplitude behavior, which yields the optimal choice for the Hamiltonian simulation time and Clock register size, with respect to the condition number of the matrix. Understanding this behavior is indispensable to extend the classical HHL error analysis to HHL variants.

II. Algorithm Details

The HHL algorithm [5], solves the matrix equation $A\boldsymbol{x} = \boldsymbol{b}$ by preparing a quantum state $|x\rangle$ proportional to the desired solution vector $\boldsymbol{x}$. Herein, we make the following assumptions for the matrix equation for simplicity:

- $A \in \mathbb{C}^{N \times N}$ is Hermitian with N being a power of 2.

- The condition number κ of A is known or can be efficiently approximated, and A is scaled so that all of its eigenvalues belong to the region $[1/\kappa, 1]$.
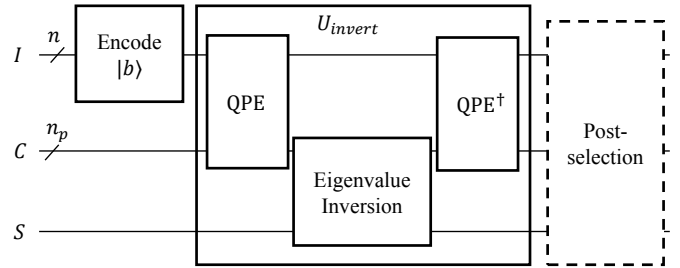- $\boldsymbol{b}$ is a normalized vector.

Fig. 1. The diagram illustration of the HHL circuit.

The diagram of the HHL circuit is given in Figure 1. Three registers are the Input/Output register I with $n = \log_2(N)$ qubits, the Clock register C with n_t qubits, and the Flag register S that contains a qutrit, whose state is spanned by basis $\{|\text{well}\rangle, |\text{ill}\rangle, |\text{nothing}\rangle\}$. We define $T := 2^{n_t}$.

The right-hand-side statevector $|b\rangle$ encoding is assumed to be carried out efficiently by some procedure, such that the initial state U_{invert} operating on is

$$|\Phi_0\rangle = |b\rangle_I |0\rangle_C |0\rangle_S = \sum_{j=0}^{N-1} \beta_j |\lambda_j\rangle_I |0\rangle_C |\text{nothing}\rangle_S, \quad (1)$$

where $|b\rangle$ is represented as $\sum_{j=0}^{N-1} \beta_j |\lambda_j\rangle$ in the eigenbasis of A: $A|\lambda_j\rangle = \lambda_j |\lambda_j\rangle$. The unitary operation U_{invert} represents the HHL procedure that inverts the matrix A. It contains three components: QPE, eigenvalue inversion, and QPE inverse, explained in the next three subsections.

A. QPE

We denote QPE as a unitary operator P, which contains three steps:

1) Prepare an initial state on register C. In accordance with HHL's formulation, the state after this step is [1]

$$|\Phi_1\rangle = \sum_{j=0}^{N-1} \beta_j |\lambda_j\rangle_I \sqrt{\frac{2}{T}}$$
$$\sum_{\tau=0}^{T-1} \sin\left[\frac{\pi}{T}\left(\tau + \frac{1}{2}\right)\right] |\tau\rangle_C |\text{nothing}\rangle_S. \quad (2)$$

2) Apply the Hamiltonian simulation (HS) $e^{iAt_0\tau/T}$ to register I conditioned on the state of the clock register $|\tau\rangle_C$. The choice of the HS time t_0 will be discussed as the outcome of Section III. The resultant state is

$$|\Phi_2\rangle = \sum_{j=0}^{N-1} \beta_j |\lambda_j\rangle_I \sqrt{\frac{2}{T}} \sum_{\tau=0}^{T-1} \sin\left[\frac{\pi}{T}\left(\tau + \frac{1}{2}\right)\right]$$
$$e^{i\lambda_j t_0\tau/T} |\tau\rangle_C |\text{nothing}\rangle_S. \quad (3)$$

3) Apply the quantum Fourier transform (QFT)

$$|\tau\rangle_C \xrightarrow{\text{QFT}} \frac{1}{\sqrt{T}} \sum_{k=0}^{T-1} e^{-i(2\pi/T)k\tau} |k\rangle_C \quad (4)$$

to register C. The resultant state is

$$|\Phi_3\rangle = \sum_{j=0}^{N-1} \beta_j |\lambda_j\rangle_I \sum_{k=0}^{T-1} \alpha_{k|j} |k\rangle_C |\text{nothing}\rangle_S, \quad (5)$$

where the amplitude is given as

$$\alpha_{k|j} = \frac{\sqrt{2}}{T} \sum_{\tau=0}^{T-1} \sin\left[\frac{\pi}{T}\left(\tau + \frac{1}{2}\right)\right] e^{i\left(\lambda_j - \frac{2\pi}{t_0}k\right)\frac{t_0}{T}\tau}. \quad (6)$$

The form of the phase term in (6) suggests the definition of the approximated eigenvalue (associated with the register C state $|k\rangle_C$) as

$$\tilde{\lambda}_k := \frac{2\pi}{t_0}k. \quad (7)$$

We further define δ_λ as the error in the eigenvalue approximation $\delta_\lambda(k|j) := \lambda_j - \tilde{\lambda}_k$.

B. Eigenvalue Inversion

QPE provides the approximated eigenvalues, the next step is to invert them, achieved by setting the a flag register S as

$$|h(\tilde{\lambda}_k)\rangle := f(\tilde{\lambda}_k)|\text{well}\rangle + g(\tilde{\lambda}_k)|\text{ill}\rangle$$
$$+ \sqrt{1 - f^2(\tilde{\lambda}_k) - g^2(\tilde{\lambda}_k)}|\text{nothing}\rangle, \quad (8)$$

where the filter functions $f(x)$ and $g(x)$ are defined as

$$f(\lambda) := \begin{cases} \frac{1}{2\tilde{\kappa}\lambda} \\ \frac{-\cos(\pi\tilde{\kappa}\lambda)}{2} \\ 0 \end{cases} \quad g(\lambda) := \begin{cases} 0, & \lambda \in \left[\frac{1}{\tilde{\kappa}}, 1\right] \\ \frac{\sin(\pi\tilde{\kappa}\lambda)}{2}, & \lambda \in \left[\frac{1}{2\tilde{\kappa}}, \frac{1}{\tilde{\kappa}}\right] \\ \frac{1}{2}, & \lambda \in \left(0, \frac{1}{2\tilde{\kappa}}\right] \end{cases} \quad (9)$$

where $\tilde{\kappa} = O(\kappa)$ is the approximated condition number.

The state after eigenvalue inversion is

$$|\Phi_4\rangle = \sum_{j=0}^{N-1} \beta_j |\lambda_j\rangle_I \sum_k \alpha_{k|j} |k\rangle_C |h(\tilde{\lambda}_k)\rangle_S. \quad (10)$$

C. QPE inverse

Apply inverse QPE $P^\dagger$, resulting in a final state $|\Phi_f\rangle$

$$|\Phi_f\rangle = P^\dagger \sum_{j=0}^{N-1} \beta_j |u_j\rangle_I \sum_{k=0}^{T-1} \alpha_{k|j} |k\rangle_C |h(\tilde{\lambda}_k)\rangle_S. \quad (11)$$

If the QPE is perfect, the final state will simplify as

$$|\Phi_f\rangle = \sum_{j=0}^{N-1} \beta_j |u_j\rangle_I |0\rangle_C |h(\lambda_j)\rangle_S. \quad (12)$$

According to (8), if we post-select (12) depending on the state of the flag register S, we will retrieve a solution state $|x\rangle$ that is proportional to the solution to the matrix equation x, provided that all eigenvalues are in the well-conditioned region $\left[\frac{1}{\kappa}, 1\right]$.

III. PHASE ESTIMATION AMPLITUDE BEHAVIORS

We define $\delta := t_0\delta_\lambda = \lambda_j t_0 - 2\pi k$, then the magnitude of the amplitude can be simplified as

$$|\alpha_{k|j}| = \frac{\sqrt{2}}{T} \sin\left(\frac{\pi}{2T}\right) \frac{\left|\cos\left(\frac{\delta}{2T}\right)\cos\left(\frac{\delta}{2}\right)\right|}{\left|\sin\left(\frac{\delta+\pi}{2T}\right)\sin\left(\frac{\delta-\pi}{2T}\right)\right|}. \quad (13)$$

QPE makes $|\alpha_{k|j}|$ approach to 1 when $|\delta_\lambda|$ is close to 0 (corresponding to a good eigenvalue approximation), and becomes a small number when $|\delta_\lambda|$ is large (corresponding to a poor eigenvalue approximation). From (7) and (13), we see that the choice of t_0 is an important factor of the eigenvalue approximation value and the corresponding approximation quality. Suppose we use the entire clock register state range, i.e., $k = 0, 1, 2, \cdots, T-1$, then the maximum approximated eigenvalue is $\max_k \tilde{\lambda}_k = \frac{2\pi(T-1)}{t_0}$.

To be able to approximate the largest eigenvalue $\frac{T-1}{T}$[2], we need to require that $\frac{2\pi(T-1)}{t_0} \geq \frac{T-1}{T}$, which indicates that $t_0 \leq 2\pi T$. The choice of $t_0 = 2\pi T$ seems a reasonable one, as the maximum eigenvalue that can be approximated is $\frac{T-1}{T}$ in this case. With such choice, the eigenvalue approximation granularity would be $1/T$. In order to ensure enough resolution of $\tilde{\lambda}_k$ point near the minimum eigenvalue $\frac{T-1}{T}\frac{1}{\kappa}$, we need to choose $T \geq \kappa + 1$. However, note that $|\alpha|$ is a continuous $2\pi T$-periodic function with respect to δ, which indicates that $k = 0$ and $k = T - 1$ gives similar amplitude magnitudes. Namely, $|\alpha(\delta(k = 0))| \approx |\alpha(\delta(k = T - 1))|$, because the input difference $\delta(k = T - 1) - \delta(k = 0) = 2\pi(T - 1)$ is close to one period. This behavior is not detrimental when the target eigenvalue λ_j is in the middle of the range (around 0.5), but when approximating small and larger eigenvalues (eigenvalues that are close to $\frac{T-1}{T}\frac{1}{\kappa}$ and $\frac{T-1}{T}$), the periodicity of $|\alpha|$ causes unwanted large amplitude at the other end of the

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[1] Herein we use the subscript to denote the register for the states and operators, e.g., U_I means a unitary operator U applied to register I, and $|u\rangle_I$ means that register I is in state $|u\rangle$.

[2] For mathematical formulation simplify, hereafter we modify the assumption on the eigenvalues' range slightly: from $[1/\kappa, 1]$ to $\frac{T-1}{T}[1/\kappa, 1]$.

approximated spectrum. Figure 2 illustrates this behavior with three instances of eigenvalues, exemplifying small, moderate, and large values.
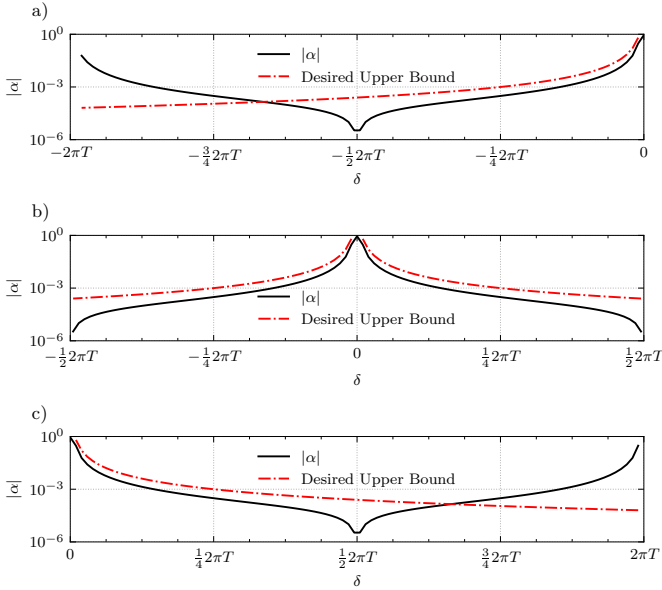

Fig. 2. $|\alpha|$ versus δ for a) small eigenvalue $\frac{T-1}{T}\frac{1}{\kappa}$, b) moderate eigenvalue $\frac{T-1}{2T}$, and c) large eigenvalue $\frac{T-1}{T}$ with $t_0 = 2\pi T, T = \kappa + 1$.

In Figure 2, we choose $t_0 = 2\pi T, T = \kappa + 1$. The tested eigenvalues are $\frac{T-1}{T}\frac{1}{\kappa}$, $\frac{T-1}{2T}$, and $\frac{T-1}{T}$ respectively. The desired upper bound for the amplitude [5] $\frac{8\pi}{\delta^2}$ is shown in the figure as well. One can perceive the continuous periodic pattern of $|\alpha|$ from these figures: the plot manifests at the opposite extremity. This is because QPE captures the periodic nature of phase: 0 and 2π are in fact the same point in the polar plane. When the actual eigenvalue is close to the left boundary $\frac{T-1}{T}\frac{1}{\kappa}$ or the right boundary $\frac{T-1}{T}$, large amplitudes appear at the poor eigenvalue approximation range. As a consequence, the desired upper bound is violated in the unwanted region of the approximated eigenvalue spectrum.

This issue can be avoided by choosing a smaller t_0, a maneuver with the side effect of wasting some range of the clock register. To explain, let us consider a choice of $t_0 = \pi T$, in which case, the approximated eigenvalues are

$$\tilde{\lambda}_k = 2\frac{k}{T} = 0, 2\frac{1}{T}, 2\frac{2}{T}, \cdots \tag{14}$$

To approximate the smallest eigenvalue, T should be at least $2\kappa + 1$. If we choose $T = 2\kappa + 1$, we only need k up to $\lceil (T-1)/2 \rceil$ to approximate the entire range of the eigenvalues, namely the clock register range is not fully used. But this waste of the clock register is inevitable to truncate half of the period of $|\alpha|$, removing the unwanted tail on the opposite side when the actual eigenvalue is close to either side of the boundary. The $|\alpha|$ versus k and δ behavior with this choice of t_0 and T is visualized in Figure 3. One can observe that the desired upper bound is not violated in the entire range of k, regardless of the actual eigenvalue.
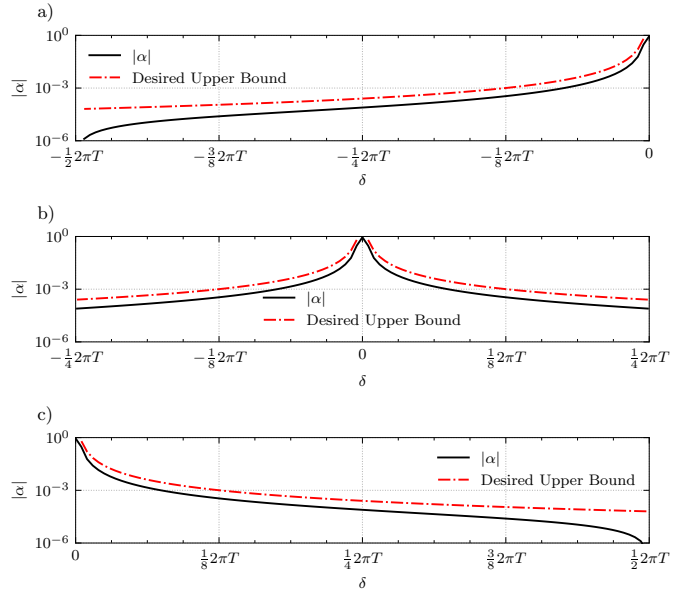

Fig. 3. Data similarly illustrated as in Figure 2 with $t_0 = \pi T, T = 2\kappa + 1$.

More generally, choosing $t_0 = c(2\pi T)$ with $c < \frac{1}{2}$ will utilize less spectrum while truncating the $|\alpha|$ more. However, as $t_0 = \frac{1}{2}(2\pi T)$ is enough to bound $|\alpha|$ in half period, choosing $c < \frac{1}{2}$ does not provide extra benefit. Hence, we find that $c = \frac{1}{2}$ is a optimal choice.

We can conclude on the choice of t_0 and T. Thanks to the analysis on the amplitude behavior, we choose $t_0 = \pi T$ and $T \geq \lceil 2\kappa + 1 \rceil$, which dictates the range of required k. According to the error analysis built on this amplitude analysis, one can see further that in practice T is chosen as $\Omega(\kappa/\epsilon)$, leading to a choice of $t_0 = O(\kappa/\epsilon)$ [5].

IV. CONCLUSION

The amplitude resulting from QPE is continuous with a $2\pi T$-periodicity with respect to δ. Because of this behavior, the Hamiltonian simulation time and the Clock register size need to be properly chosen, such that the QPE granularity is sufficient, simultaneously removing the unwanted tail. Accordingly, the range of k, the Clock register state is determined. The optimal choice is provided, and the logic of the optimity of such choice is given. As a future work, this analysis will be applied to the error analysis of [4].

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