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PHASE ESTIMATION USING AN APPROXIMATE EIGENSTATE

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A basic building block of many quantum algorithms is the Phase Estimation algorithm (PEA). It finds an eigenphase ϕ of a unitary operator using a copy of the corresponding eigenstate $|\phi\rangle$. Suppose, in place of $|\phi\rangle$, we have a copy of an approximate eigenstate $|\psi\rangle$ whose component in $|\phi\rangle$ is at least $\sqrt{2/3}$. Then the PEA fails with a constant probability. Using multiple copies of $|\psi\rangle$, this probability can be made to decrease exponentially with the number of copies. Here we show that a single copy is sufficient to find ϕ if we can selectively invert the $|\psi\rangle$ state. As an application, we consider the eigenpath traversal problem (ETP) where the goal is to travel a path of non-degenerate eigenstates of n different operators. The fastest algorithm for ETP is due to Boixo, Knill and Somma (BKS) which needs $\Theta(\ln n)$ copies of the eigenstates. Using our method, the BKS algorithm can work with just a single copy but its running time $\mathcal{Q}$ increases to $O(\mathcal{Q}\ln^2\mathcal{Q})$. This tradeoff is beneficial if the spatial resources are more constrained than the temporal resources.

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1 Introduction

The Phase estimation algorithm (PEA) is the backbone of many important quantum algorithms [1, 2, 3, 4]. It estimates the eigenvalues of an operator using a copy of the corresponding eigenstate. Let $|\phi\rangle$ be an eigenstate of a unitary operator U with the eigenvalue $e^{i2\pi\phi}$. The PEA uses μ ancilla qubits whose Hilbert space has the basis states $|k\rangle$ ($k \in \{0, 1, \ldots, 2^\mu - 1\}$). The initial state of the PEA is $|\phi\rangle|0_\mu\rangle$ where $|0_\mu\rangle$ denotes the state of all μ ancilla qubits in the $|0\rangle$ state. This initial state is transformed to $|\phi\rangle|f(\phi)\rangle$ where $|f(\phi)\rangle$ estimates ϕ as its measurement yields only those $|k\rangle$'s with non-negligible probabilities for which k is within a narrow interval of constant size centered at $k(\phi) = \lfloor 2^\mu\phi \rfloor$. The PEA achieves this transformation by applying an operator $\mathcal{E}(U)$ which needs 2^μ applications of U.

Consider a variant of the PEA where we don't have a perfect eigenstate $|\phi\rangle$ but an approximate one $|\psi\rangle$ which satisfies $|\langle\psi|\phi\rangle| = \alpha \geq \sqrt{2/3}$. Let PEA$\approx$ denote this variant of the PEA. If we simply use the PEA for this variant then $|\psi\rangle|0_\mu\rangle$ gets transformed by $\mathcal{E}(U)$ to $|\psi, f\rangle = \alpha|\phi\rangle|f(\phi)\rangle + |\perp\rangle|\#\rangle$ where $\langle\phi|\perp\rangle$ is zero and $|\#\rangle$ is some state of ancilla qubits. The component of $|\psi, f\rangle$ in $|f(\phi)\rangle$ is α so ϕ can be estimated with a probability of $\alpha^2 \geq \frac{2}{3}$ and the error probability can be as high as $\frac{1}{3}$. The PEA$\approx$ aims to reduce this error probability for which several methods can be used.

The simplest method is the *multiple-repititions-method* (MRM) which works as long as the approximate eigenstate $|\psi\rangle$ is easy to prepare. Starting with a copy of $|\psi\rangle$, we apply the PEA to get the state $\alpha|\phi\rangle|f(\phi)\rangle + |\perp\rangle|\#\rangle$ after which we measure the ancilla qubits. Assuming that we can reliably distinguish between $|f(\phi)\rangle$ and $|\#\rangle$, ϕ can be estimated with a success probability of $\alpha^2 \geq \frac{2}{3}$. If we succeed then we stop else we prepare another copy of $|\psi\rangle$ and repeat the process. The failure probability of a single process is $(1-\alpha^2) \leq \frac{1}{3}$ and after r repititions, this failure probability reduces exponentially as $(1-\alpha^2)^r$. The expected number of repititions required for the success is $1/\alpha^2 \leq \frac{3}{2}$ which is $\Theta(1)$.

However, in general, a reliable distinction between $|f(\phi)\rangle$ and $|\#\rangle$ is not possible as it requires a prior estimate of $|f(\phi)\rangle$ and hence ϕ which is not available (in fact, we try to find it using the PEA$\approx$). Then the only way is to repeat the PEA r times (which involves r sequential preparations of $|\psi\rangle$) and to keep track of all r measurement outcomes. The probability of getting $|f(\phi)\rangle$ in a single measurement is $\alpha^2 \geq \frac{2}{3}$ so the expected number of measurements yielding $|f(\phi)\rangle$ is at least $\frac{2}{3}r$. Due to Hoeffding's bound [5], the probability of getting $|f(\phi)\rangle$ in less than $\frac{r}{2}$ measurements is at most $e^{-2rt^2} = e^{-\Theta(r)}$ where $t = \frac{2}{3} - \frac{1}{2} = \frac{1}{6}$. Hence more than $\frac{r}{2}$ measurements yield $|f(\phi)\rangle$ with a probability of $1 - e^{-\Theta(r)} \approx 1$ for sufficiently large r. This allows us to estimate ϕ as the measurement of $|f(\phi)\rangle$ outputs only those k's which are within a narrow interval centered at $k(\phi) = \lfloor 2^\mu \phi \rfloor$. If an algorithm uses n instances of the PEA$\approx$ then its success demands $e^{-\Theta(r)} \ll \frac{1}{n}$ and hence $r = \Theta(\ln n)$ sequential preparations of $|\psi\rangle$.

Suppose $|\psi\rangle$ is not so easy to prepare so that r times sequential preparations of $|\psi\rangle$ are not feasible. Then we can use the *multiple-copies-method* (MCM) which assumes access to r parallel copies of $|\psi\rangle$. With each copy, we attach a register of μ ancilla qubits. We do r parallel applications of $\mathcal{E}(U)$ to get $|\psi, f\rangle^{\otimes r}$ which can be written as $\chi_>|\ >\rangle + \chi_<|\ <\rangle$. Here $|\ >\rangle$ ($|\ <\rangle$) is a normalized state in which more (less) than $\frac{r}{2}$ registers are in $|f(\phi)\rangle$. The probability of getting a single register in $|f(\phi)\rangle$ is $\alpha^2 \geq \frac{2}{3}$ so the expected number of registers in $|f(\phi)\rangle$ is at least $\frac{2}{3}r$. Due to Hoeffding's bound [5], the probability of getting less than $\frac{r}{2}$ registers in $|f(\phi)\rangle$ is at most e^{-2rt^2} where $t = \frac{2}{3} - \frac{1}{2} = \frac{1}{6}$ and hence $\chi_< = e^{-\Theta(r)}$. It is easy to distinguish between the $|\ >\rangle$ and $|\ <\rangle$ states by reversibly determining whether more than half registers are in $|f(\phi)\rangle$ or not. This measures $|\psi, f\rangle^{\otimes r}$ in the $\{|\ >\rangle, |\ <\rangle\}$ basis to yield $|\ >\rangle$ with a probability of $1 - \chi_<^2$. Then $k(\phi)$ can be reversibly computed to estimate ϕ. After this, r parallel applications of $[\mathcal{E}(U)]^\dagger$ on $|\ >\rangle$ yield the state $(|\psi\rangle|0_\mu\rangle)^{\otimes r} + |\chi_<\rangle$, where $|\chi_<\rangle$ has a length of $\chi_<$. As desired, all r copies of $|\psi\rangle$ remain intact up to an error term $O(\chi_<)$ which is $e^{-\Theta(r)}$. If an algorithm uses n instances of the PEA$\approx$ then its success demands $\chi_< \ll \frac{1}{n}$ and hence $r = \Theta(\ln n)$ copies of $|\psi\rangle$.

In this paper, we present a different method for the PEA$\approx$ with some advantageous features. We refer to our method as the *multiple-selective-inversions-method* (MSIM). The MSIM only requires easy implementations of the selective phase inversion of $|\psi\rangle$, i.e. $R_\psi = \mathbb{1} - 2|\psi\rangle\langle\psi|$. This is always less demanding than the easy preparations of $|\psi\rangle$ as required by the MRM. Also, the MSIM works using only a single copy of $|\psi\rangle$, unlike the MCM which needs multiple copies. The paper is organized as following. In the next section, we motivate our readers by presenting an important application of our method to the Eigenpath Traversal Problem. In Section 3, we present an overlap detection subroutine $\mathcal{S}$ used by our method which is presented in Section 4. We discuss and conclude in Section 5.

2 Motivation

Our method finds an important application in the Eigenpath Traversal Problem (ETP) which may be considered as a digital analogue of the quantum adiabatic evolution [6, 7]. It has important applications ranging from quantum physics simulation to optimization problems as discussed in detail in [8]. In the ETP, we have a path of nondegenerate eigenstates $|\theta_s\rangle$ of operators V_s with the eigenvalues $e^{i2\pi\theta_s}$ for $s \in \{1, 2, \ldots, n\}$. For any s, the eigenphase θ_s has a minimum spectral gap of Δ from non-θ_s eigenphases of V_s. The goal is to evolve $|\theta_1\rangle$ to $|\theta_n\rangle$ using minimum number of applications of the operators V_s. The best algorithm for the ETP is due to Boixo, Knill, and Somma (BKS) [6] which is a sequence of $n-1$ transformations $\mathcal{T}_s = |\theta_s\rangle \rightarrow |\theta_{s+1}\rangle$ for $s \in \{1, 2, \ldots, n-1\}$ starting with $s = 1$. Assuming $|\langle\theta_s|\theta_{s+1}\rangle|^2 \geq \frac{1}{3}$, the transformation $\mathcal{T}_s$ is implemented using a fixed-point quantum search algorithm [9, 10] which needs $\Theta(1)$ applications of the selective phase inversions $R_{\theta,s}$ and $R_{\theta,s+1}$ where $R_{\theta,s} = \mathbb{1} - 2|\theta_s\rangle\langle\theta_s|$ and similarly for $R_{\theta,s+1}$ (Theorem V.1 of [6]).

The BKS algorithm does not need any kind of phase estimation algorithms (PEA or PEA$\approx$) if we have a prior knowledge of the eigenphases θ_s up to an accuracy of $\frac{\Delta}{4}$. Using this prior knowledge, the operator $R_{\theta,s}$ can be implemented using $\frac{1}{\Delta}\Theta(\ln\frac{1}{\epsilon_0})$ applications of V_s where ϵ_0 is the desired error probability (see [11], Definition III.3 of [6] and Section III of [12]). As the BKS algorithm uses $\Theta(n)$ implementations of $R_{\theta,s}$, we must choose $\epsilon_0 = \Theta(\frac{1}{n})$ to be successful. Hence we need $\mathcal{Q} = \Delta^{-1}\Theta(n \ln n)$ applications of V_s which is the time complexity of the BKS algorithm. Also, Lemma V.3 of [6] shows that another sequence of eigenstates $|\theta'_s\rangle$ can be found such that $|\theta'_1\rangle = |\theta_1\rangle$ and $|\theta'_{n'}\rangle = |\theta_n\rangle$, where $n' = O(L) \leq n$. Here L is the *angular path length* whose value is $\sup\left(\sum_{s=1}^{n} \cos^{-1}|\langle\theta_s|\theta_{s-1}\rangle|\right)$. Thus the time complexity becomes $\frac{1}{\Delta}\Theta(L \ln L)$ which is better than $\Theta(L^2/\Delta)$, the complexity of a previous algorithm based on phase randomization [8]. It has been proved that the optimal time complexity is $\Theta(L/\Delta)$ [13].

More generally, we don't have any prior knowledge of the eigenphases θ_s. In such situations, we must use the phase estimation algorithms to estimate θ_s so that $R_{\theta,s}$ can be implemented. Suppose we have somehow obtained a copy of $|\theta_s\rangle$ and now we want to transform it to $|\theta_{s+1}\rangle$ using the transformation $\mathcal{T}_s$. As mentioned earlier, $\mathcal{T}_s$ uses $\Theta(1)$ applications of both $R_{\theta,s}$ and $R_{\theta,s+1}$. Using the available copy of $|\theta_s\rangle$, the PEA can be used to estimate θ_s up to an accuracy of $O(\Delta)$ using $O(\frac{1}{\Delta})$ applications of V_s. This estimate can be used then to implement $R_{\theta,s}$. The question is: how do we implement another necessary transformation $R_{\theta,s+1}$ which requires an estimate of θ_{s+1}. The PEA cannot be used to estimate θ_{s+1} as, unlike $|\theta_s\rangle$, we don't have a copy of the $|\theta_{s+1}\rangle$ state. In fact, $|\theta_{s+1}\rangle$ is the final state of the desired transformation $\mathcal{T}_s$. To overcome this problem, the BKS algorithm assumes $|\langle\theta_s|\theta_{s+1}\rangle|^2 \geq \frac{2}{3}$ (Theorem V.2 of [6]) for all s so that $|\theta_s\rangle$ can serve as an approximate eigenstate for the operator V_{s+1}. Then the PEA$\approx$ algorithms can use the available copy of $|\theta_s\rangle$ to estimate θ_{s+1}. The estimates of both θ_s and θ_{s+1} enable us to implement $R_{\theta,s}$ and $R_{\theta,s+1}$ respectively and hence to implement the desired transformation $\mathcal{T}_s$.

The BKS algorithm becomes highly inefficient if we use the simplest multiple-repitition-method (MRM) for the PEA$\approx$. The initial state is $|\theta_1\rangle$. We need r times preparations of $|\theta_1\rangle$ for a single preparation of $|\theta_2\rangle$, r times preparations of $|\theta_2\rangle$ (which needs r^2 times preparations of $|\theta_1\rangle$) are needed for a single preparation of $|\theta_3\rangle$ and so on. Thus we need $r^{s'}$ preparations of $|\theta_s\rangle$ for a single preparation of $|\theta_{s+s'}\rangle$. To get $|\theta_n\rangle$, we need a total of r^{n-1} times preparations

of $|\theta_1\rangle$ and as $r = \Theta(\ln n)$, the time complexity is exponential in n and hence highly inefficient. This exponential complexity is true even if we can somehow distinguish between $|f(\phi)\rangle$ and $|\#\rangle$ states as mentioned in Section 1. Then the expected number of preparations of $|\theta_s\rangle$ for a single preparation of $|\theta_{s+1}\rangle$ is $1/\alpha^2 \leq \frac{3}{2}$. Hence the time complexity can be as high as $(3/2)^n$. We note that the MRM method fails miserably in the case of the BKS algorithm only because it assumes easy preparations of $|\psi\rangle$. This assumption becomes very costly if many sequential applications of the PEA$\approx$ are required as in the BKS algorithm.

To overcome this problem, the BKS algorithm uses the method of multiple copies (MCM) of $|\theta_1\rangle$. As it uses $\Theta(n)$ instances of the PEA$\approx$, we need $r = \Theta(\ln n)$ copies of $|\theta_1\rangle$. These r copies of $|\theta_1\rangle$ are transformed to r copies of $|\theta_2\rangle$, which are then transformed to r copies of $|\theta_3\rangle$ and so on. This process continues till we get r copies of the desired final state $|\theta_n\rangle$. Using the MCM, the BKS algorithm works using $\mathcal{Q} = \Delta^{-1}\Theta(n \ln n)$ applications of V_s and as discussed earlier, this is same as the case when we have a prior estimate of the eigenphases θ_s. The only problem is that we need a parallel processing on $\Theta(\ln n)$ copies of the eigenstates and this adds to the burden on the spatial resources.

We present our method of the MSIM to address the problem of spatial resources. Using the MSIM, the BKS algorithm can work using just a single copy of the initial state $|\theta_1\rangle$. As mentioned earlier, the MSIM uses multiple applications of the selective phase inversions of the approximate eigenstate $|\psi\rangle$ to get an estimate of ϕ. In the case of the BKS algorithm, we need to implement a series of $n-1$ transformations $\mathcal{T}_s$ which use $R_{\theta,s}$ and $R_{\theta,s+1}$ to transform an available copy of $|\theta_s\rangle$ to a desired copy of $|\theta_{s+1}\rangle$. As $|\theta_s\rangle$ is an exact eigenstate of V_s, the PEA can be used to estimate θ_s which enables us to implement $R_{\theta,s}$. This implementation of $R_{\theta,s}$ can be used in our method of the MSIM to estimate θ_{s+1} as the assumption $|\langle\theta_s|\theta_{s+1}\rangle|^2 \geq \frac{2}{3}$ makes $|\theta_s\rangle$ to serve as an approximate eigenstate of V_{s+1}. The estimate of θ_{s+1} enables us to implement $R_{\theta,s+1}$ which, alongwith the implementation of $R_{\theta,s}$, allows us to implement the desired transformation $\mathcal{T}_s$.

However, the cost of using multiple selective inversions is that the time complexity increases from $\mathcal{Q}$ to $O(\mathcal{Q}\ln^2\mathcal{Q})$. This space-time tradeoff is beneficial if the spatial resources are more constrained than the temporal resources. Typically $\mathcal{Q} \gg 1$ and increasing the time from $\mathcal{Q}$ to $O(\mathcal{Q}\ln^2\mathcal{Q})$ is not a big concern if doing so removes the necessity of $\Theta(\ln n)$ copies of the eigenstates. For example, a 50-qubit quantum computer can handle larger quantum systems using our method. Next, we present an overlap detection subroutine used by our method.

3 Overlap Detection Subroutine

In this section, we present an Overlap Detection Subroutine $\mathcal{S}$ to detect if the overlap magnitude of an unknown quantum state $|\sigma\rangle$ with a known subspace is at least $\sqrt{4/9}$ or less than $\sqrt{5/9}$. Both of these inequalities may be true, but detecting only one is sufficient for our purpose. Let $|\lambda\rangle$ and $|\lambda^\perp\rangle$ denote the projections of $|\sigma\rangle$ on mutually complementary subspaces Λ and $\Lambda^\perp$ respectively. Then

$$|\sigma\rangle = \sin\omega|\lambda\rangle + \cos\omega|\lambda^\perp\rangle, \quad P_\lambda(\sigma) = \sin^2\omega, \tag{1}$$

where $P_\lambda(\sigma)$ is the probability of getting $|\lambda\rangle$ after measuring $|\sigma\rangle$. We wish to detect if $P_\lambda(\sigma) \geq \frac{4}{9}$ or $P_\lambda(\sigma) < \frac{5}{9}$.

The previous overlap detection subroutines are based on the quantum amplitude amplification [14] to estimate $\sin\omega$. But they don't preserve the $|\sigma\rangle$ state with sufficiently high probability. For example, the subroutine used by the BKS algorithm (Definition III.4 of [6]) preserves $|\sigma\rangle$ while detecting if $\sin\omega < \eta_0 - \eta$ or $\sin\omega > \eta_0 + \eta$. But it fails if $\sin\omega \in [\eta_0 - \eta, \eta_0 + \eta]$. Choosing a small η increases the time complexity as $O(\frac{1}{\eta})$ and a careful calculation shows that the time complexity becomes significantly large in case when multiple estimations are needed.

Preserving the $|\sigma\rangle$ state is crucial for our purpose. Our subroutine $\mathcal{S}$ does it with a sufficiently high probability. It becomes simpler if $P_\lambda(\sigma)$ can be lower bounded. This is done by attaching an ancilla qubit in the state $\frac{1}{\sqrt{10}}(|0\rangle + 3|1\rangle)$ to $|\sigma\rangle$. The joint state is

$$\sqrt{10}|\sigma'\rangle = \sin\omega|0\lambda\rangle + \cos\omega|0\lambda^\perp\rangle + 3\sin\omega|1\lambda\rangle + 3\cos\omega|1\lambda^\perp\rangle. \tag{2}$$

Let $|\lambda'\rangle$ be the projection of $|\sigma'\rangle$ on the subspace Λ' spanned by $\{|0\lambda\rangle, |0\lambda_\perp\rangle, |1\lambda\rangle\}$. Then

$$|\sigma'\rangle = \sin\omega'|\lambda'\rangle + \cos\omega'|\lambda'^\perp\rangle, \quad P'_\lambda(\sigma) = \sin^2\omega' = (9/10)P_\lambda(\sigma) + (1/10). \tag{3}$$

Here $|\lambda'^\perp\rangle$ is orthogonal to $|\lambda'\rangle$. Thus $P'_\lambda(\sigma) \geq 1/10$ as desired. Also,

$$P_\lambda(\sigma) \geq 4/9 \Longrightarrow P'_\lambda(\sigma) \geq 5/10, \quad P_\lambda(\sigma) < 5/9 \Longrightarrow P'_\lambda(\sigma) < 6/10. \tag{4}$$

Thus, for our purpose, we need to detect if $P'_\lambda(\sigma) \geq \frac{5}{10}$ or $P'_\lambda(\sigma) < \frac{6}{10}$.

Consider the amplitude amplification operator $\mathcal{A} = R_{\sigma'}R_{\lambda'}$, where R_ϑ is $\mathbb{1} - 2|\vartheta\rangle\langle\vartheta|$, the selective inversion of $|\vartheta\rangle$. To implement $R_{\lambda'}$, we invert the Λ' subspace. First, we apply the single qubit gate $-Z = R_0$ on the ancilla qubit to invert $|0\lambda\rangle$ and $|0\lambda^\perp\rangle$. Then, to invert $|1\lambda\rangle$, we apply R_λ if and only if the ancilla qubit is in the $|1\rangle$ state. To implement $R_{\sigma'}$, let C be a single qubit gate such that $|\sigma'\rangle = C|0\sigma\rangle$. Then $R_{\sigma'} = CR_{0\sigma}C^\dagger$ where $R_{0\sigma}$ is implemented by applying R_σ if and only if the ancilla qubit is in the $|0\rangle$ state. The eigenspectrum of $\mathcal{A}$ has been analysed in Section 2 of [14]. It is shown there that

$$\mathcal{A}|\Omega_\pm\rangle = e^{\pm i2\omega'}|\Omega_\pm\rangle, \quad \sqrt{2}|\Omega_\pm\rangle = |\lambda'\rangle \pm |\lambda'^\perp\rangle, \quad \sqrt{2}|\sigma'\rangle = e^{i\omega'}|\Omega_+\rangle - e^{-i\omega'}|\Omega_-\rangle. \tag{5}$$

Consider a state $|\kappa\rangle$ satisfying $|\langle\kappa|\Omega_\pm\rangle| = \frac{1}{\sqrt{2}}$. We attach an ancilla qubit and start with

$$2|\kappa\rangle|+\rangle = e^{i\kappa_+}|\Omega_+\rangle|0\rangle + e^{i\kappa_+}|\Omega_+\rangle|1\rangle + e^{i\kappa_-}|\Omega_-\rangle|0\rangle + e^{i\kappa_-}|\Omega_-\rangle|1\rangle. \tag{6}$$

We apply $\mathcal{A}$ on $|\kappa\rangle$ if the ancilla qubit is in the $|1\rangle$ state. Up to a factor of 2, we get

$$e^{i\kappa_+}|\Omega_+\rangle\left(|0\rangle + e^{i2\omega'}|1\rangle\right) + e^{i\kappa_-}|\Omega_-\rangle\left(|0\rangle + e^{-i2\omega'}|1\rangle\right). \tag{7}$$

We apply the Hadamard gate H on the ancilla qubit. Up to a factor of $\sqrt{2}$, we get

$$\left(e^{i(\kappa_+ + \omega')}|\Omega_+\rangle + e^{i(\kappa_- - \omega')}|\Omega_-\rangle\right)\cos\omega'|0\rangle - i\left(e^{i(\kappa_+ + \omega')}|\Omega_+\rangle - e^{i(\kappa_- - \omega')}|\Omega_-\rangle\right)\sin\omega'|1\rangle.$$

Measuring the ancilla qubit yields the $|\kappa + 1\rangle$ state. The probabilities of outcomes X_κ are

$$\mathrm{Prob(X_\kappa = 1)} = \sin^2\omega' = \mathrm{P'_\lambda(\sigma)}, \quad \mathrm{Prob(X_\kappa = 0)} = 1 - \mathrm{P'_\lambda(\sigma)}. \tag{8}$$

It is easy to check that $(\kappa+1)_+ = \kappa_+ + \omega'$ and $(\kappa+1)_- = \kappa_- - \omega' + \pi X_\kappa$, so

$$\sqrt{2}|\kappa+1\rangle = e^{i(\kappa_+ + \omega')}|\Omega_+\rangle + (-1)^{X_\kappa} e^{i(\kappa_- - \omega')}|\Omega_-\rangle. \tag{9}$$

We iterate this process q times to get the state $|\kappa+q\rangle$ for which

$$(\kappa+q)_+ = \kappa_+ + q\omega', \quad (\kappa+q)_- = \kappa_- - q\omega' + \pi(N_1 \mathrm{mod} 2). \tag{10}$$

Here $N_1 = \sum_\kappa^{\kappa+q-1} X_\kappa$ is the total number of 1's as measurement outcomes during q iterations. In a single iteration, the measurement probability of getting 1 is $P'_\lambda(\sigma)$ due to Eq. (8). Hence N_1 has a binomial probability distribution having a sharp peak at $N_1^{\max} = qP'_\lambda(\sigma)$ and decaying exponentially away from $N_1^{\max}$. Quantitatively, Hoeffding's bound [5] implies

$$\mathrm{Prob}\left(|\mathrm{N}_1 - \mathrm{N}_1^{\max}|/\mathrm{q} > \mathrm{t}\right) = \mathrm{Prob}\left(|(\mathrm{N}_1/\mathrm{q}) - \mathrm{P}'_\lambda(\sigma)| > \mathrm{t}\right) \leq \mathrm{e}^{-2\mathrm{qt}^2}. \tag{11}$$

Thus, with the error probability $e^{-q/200}$, the value of N_1 detects $P'_\lambda(\sigma)$ as

$$N_1 \geq 0.55q \Longrightarrow P'_\lambda(\sigma) \geq 0.5, \qquad N_1 < 0.55q \Longrightarrow P'_\lambda(\sigma) < 0.6. \tag{12}$$

To get back the $|\kappa\rangle$ state, we choose q to be even. If N_1 is also even then Eqs. (5) and (10) imply that $|\kappa+q\rangle = \mathcal{A}^{q/2}|\kappa\rangle$ and $|\kappa\rangle$ is obtained by $\frac{q}{2}$ applications of $\mathcal{A}^\dagger$ on $|\kappa+q\rangle$. If N_1 is odd, we choose $q = q+2$ by adding 2 extra iterations. It keeps q even and N_1 remains odd only if X_κ's are $\{0,0\}$ or $\{1,1\}$ in extra iterations, the probability of which is $1 - 2P'_\lambda(\sigma)[1 - P'_\lambda(\sigma)] \leq 0.82 = 0.91^2$ as $P'_\lambda(\sigma) \geq \frac{1}{10}$. We keep on adding extra iterations till N_1 becomes even. The error probability of N_1 remaining odd after q_e extra iterations is at most $0.91^{q_e} < e^{-0.09q_e}$. Choosing $q_e = q/10$, this is negligible compared to the error probability $e^{-q/200}$ of Eq. (12). Hence $q + q_e = 1.1q$ iterations reduce the error probability to $e^{-q/200}$. If ϵ_1 is the desired error probability then we must choose $q = \Theta(\ln \frac{1}{\epsilon_1})$. Thus, if the initial state $|\kappa\rangle$ is $|\sigma\rangle$ then the subroutine $\mathcal{S}$ needs $\frac{3q}{2} = \Theta(\ln \frac{1}{\epsilon_1})$ applications of $\mathcal{A}$: q for q iterations and $\frac{q}{2}$ to get back the $|\sigma\rangle$ state. This subroutine $\mathcal{S}$ is used by our method which is presented in the next section.

4 Method of Multiple Selective Inversions (MSIM)

In this section, we present our method of phase estimation algorithm using an approximate eigenstate $|\psi\rangle$. We define the operators U_γ having $|\phi\rangle$ as their eigenstate with the eigenvalue $e^{i2\pi\phi_\gamma}$, i.e.

$$U_\gamma = U^{2^\gamma} \Longrightarrow U_\gamma|\phi\rangle = e^{i2\pi\phi_\gamma}|\phi\rangle, \quad \phi_\gamma = 2^\gamma\phi. \tag{13}$$

We choose $\mu = 5$ and work in the Hilbert space $\mathcal{H}_J = \mathcal{H}_m \otimes \mathcal{H}_{32}$. Here $\mathcal{H}_m$ is the Hilbert space spanned by the eigenstates of U and $\mathcal{H}_{32}$ is the Hilbert space of 5 ancilla qubits. Each basis state $|k\rangle$ of $\mathcal{H}_{32}$ encodes an integer $k \in \{0,1,\ldots,31\}$ which is the decimal value of the binary number encoded by $|k\rangle$. The PEA operator $\mathcal{E}(U_\gamma)$ transforms $|\phi\rangle|0_\mu\rangle$ to $|\phi\rangle|f_\gamma\rangle$ where $|f_\gamma\rangle$ estimates ϕ_γ. To quantify this estimate, let $[a,b]$ be the set of integers ranging from a to b in the increasing order modulo 32. For example, $[16,15]$ is the set $\{16,17,\ldots,31,0,\ldots,15\}$, not $\{16,15\}$. Let $[a \pm c]$ be the set $[a-c, a+c]$. Let Λ_a^b be the subspace of $\mathcal{H}_J$ in which $|k\rangle$ satisfy $k \in [a,b]$ and let Π_a^b be the projection operator on Λ_a^b. For any state $|\sigma\rangle$ in $\mathcal{H}_J$, the probability $P_a^b(\sigma)$ of getting an integer $k \in [a,b]$ after measurement is

$$P_a^b(\sigma) = |\langle\sigma|\lambda_a^b(\sigma)\rangle|^2, \quad |\lambda_a^b(\sigma)\rangle = \Pi_a^b|\sigma\rangle. \tag{14}$$

In our notation, Eq. (5.34) of [2] (based on the analysis of [3]) can be written as

$$P_{k(\phi_\gamma)\pm c}(\phi, f_\gamma) = P^{k(\phi_\gamma)+c}_{k(\phi_\gamma)-c}(\phi, f_\gamma) \geq 1 - [2(c-1)]^{-1}, \quad k(\phi_\gamma) = \lfloor 32\phi_\gamma \rfloor, \quad c > 1. \tag{15}$$

With the choice $c = 4$, we find that $P_{k(\phi_\gamma)\pm 4}(\phi, f_\gamma)$ is at least $\frac{5}{6}$.

For an approximate eigenstate $|\psi\rangle|0_\mu\rangle$ is transformed by $\mathcal{E}(U_\gamma)$ to $|\psi, f_\gamma\rangle = \alpha|\phi\rangle|f(\phi_\gamma)\rangle + |\perp\rangle|\#\rangle$ where $\langle\phi|\perp\rangle = 0$ due to which $|\perp\rangle|\#\rangle$ only adds to the probabilities of getting any k. Thus

$$P_{k(\phi_\gamma)\pm 4}(\psi, f_\gamma) \geq \alpha^2 P_{k(\phi_\gamma)\pm 4}(\phi, f_\gamma) \geq (2/3) \times (5/6) = (5/9). \tag{16}$$

Let $\mathrm{M}_\gamma[\mathrm{x}]$ be the $(\gamma+1)^{\mathrm{th}}$ most significant bit of x. Then Eqs. (13) and (15) imply

$$\mathrm{M}_{\gamma'}[\phi_\gamma] = \mathrm{M}_{\gamma+\gamma'}[\phi], \quad \gamma \leq 4 \Longrightarrow \mathrm{M}_\gamma[\mathrm{k}(\phi_\gamma)] = \mathrm{M}_\gamma[\phi_\gamma]. \tag{17}$$

If $k(\phi_\gamma) \in [0, 7]$ then $[k(\phi_\gamma) \pm 4] \subset [28, 11]$. As $[a, b] \subset [a', b']$ implies $P^{b'}_{a'}(\sigma) \geq P^b_a(\sigma)$, we get

$$k(\phi_\gamma) \in [0, 7] \Longrightarrow P^{11}_{28}(\psi, f_\gamma) \geq 5/9, \quad P^{11}_{28}(\psi, f_\gamma) < 5/9 \Longrightarrow k(\phi_\gamma) \notin [0, 7], \tag{18}$$

where we have used Eq. (16). Relabeling the basis states as $|k\rangle \longrightarrow |(k+16)\mathrm{mod}32\rangle$, we get $P^{27}_{12}(\psi, f_\gamma) < 5/9 \Longrightarrow k(\phi_\gamma) \notin [16, 23]$. By definition, $P^{27}_{12}(\sigma) + P^{11}_{28}(\sigma) = 1$. Hence

$$P^{27}_{12}(\psi, f_\gamma) \geq 4/9 \Longrightarrow k(\phi_\gamma) \notin [0, 7], \quad P^{27}_{12}(\psi, f_\gamma) < 5/9 \Longrightarrow k(\phi_\gamma) \notin [16, 23]. \tag{19}$$

Relabeling the basis states again as $|k\rangle \longrightarrow |(k+8)\mathrm{mod}32\rangle$, we get

$$P^3_{20}(\psi, f_\gamma) \geq 4/9 \Longrightarrow k(\phi_\gamma) \notin [8, 15], \quad P^3_{20}(\psi, f_\gamma) < 5/9 \Longrightarrow k(\phi_\gamma) \notin [24, 31]. \tag{20}$$

These relations are summarized in Table 1 where $P_{0\gamma} \equiv P^{27}_{12}(\psi, f_\gamma)$ and $P_{1\gamma} \equiv P^3_{20}(\psi, f_\gamma)$. The entries of column G are easy to check. For example, $k(\phi_\gamma) \notin [0, 7]$ and $k(\phi_\gamma) \notin [24, 31]$ imply $k(\phi_\gamma) \in [8, 23]$ and $\mathrm{M}_0[\mathrm{k}(\phi_\gamma)] = 1 - \mathrm{M}_1[\mathrm{k}(\phi_\gamma)]$. To get the entries of column H, we have used Eq. (17).

Table 1. Finding the most significant bits of ϕ using the values of $P_{0\gamma}$ and $P_{1\gamma}$.

A	B	C	D	E	F	G	H
Case	$P_{0\gamma}$	$k(\phi_\gamma) \notin$	$P_{1\gamma}$	$k(\phi_\gamma) \notin$	$k(\phi_\gamma) \in$	$\mathrm{M}_0[\mathrm{k}(\phi_\gamma)]$	$\mathrm{M}_\gamma[\phi]$
1	$\geq 4/9$	[0,7]	$\geq 4/9$	[8, 15]	[16, 31]	1	1
2	$\geq 4/9$	[0, 7]	$< 5/9$	[24, 31]	[8, 23]	$1 - \mathrm{M}_1[\mathrm{k}(\phi_\gamma)]$	$1 - \mathrm{M}_{\gamma+1}[\phi]$
3	$< 5/9$	[16, 23]	$\geq 4/9$	[8, 15]	[24, 7]	$\mathrm{M}_1[\mathrm{k}(\phi_\gamma)]$	$\mathrm{M}_{\gamma+1}[\phi]$
4	$< 5/9$	[16, 23]	$< 5/9$	[24, 31]	[0, 15]	0	0

Let $\mathcal{S}_{g\gamma}$ ($g \in \{0, 1\}$) denote the overlap detection subroutine $\mathcal{S}$ to determine if $P_{g\gamma} \geq \frac{4}{9}$ or $P_{g\gamma} < \frac{5}{9}$. To estimate ϕ, we start with $\gamma = 0$ and find either $\mathrm{M}_0[\phi]$ or its value in terms of $\mathrm{M}_1[\phi]$. We increase γ by 1 and find either $\mathrm{M}_1[\phi]$, which also determines $\mathrm{M}_0[\phi]$, or the value of $\mathrm{M}_1[\phi]$ in terms of $\mathrm{M}_2[\phi]$. We keep on increasing γ by 1 till $\gamma = \Gamma$ when we find either $\mathrm{M}_\Gamma[\phi]$ in cases $(1, 4)$, which also determines $\mathrm{M}_\gamma[\phi]$ for all $\gamma < \Gamma$, or we find the value of $\mathrm{M}_\Gamma[\phi]$ in terms of $\mathrm{M}_{\Gamma+1}[\phi]$ in cases $(2, 3)$. Suppose case 2 is true and $k(\phi_\Gamma) \in [8, 23]$. We define U^+ as $U^+|\phi\rangle = e^{i2\pi\phi^+}|\phi\rangle$ where ϕ^+ is $\phi + 2^{-\Gamma-2}$. Thus $\phi^+_\Gamma = \phi_\Gamma + 0.25$ and $k(\phi^+_\Gamma) = k(\phi_\Gamma) + 8 \in [16, 31]$ implying $\mathrm{M}_\Gamma[\phi^+] = 1$. Similarly, $\mathrm{M}_\Gamma[\phi^+] = 0$ if case 3 is true. So

we find either $\mathrm{M}_\Gamma[\phi^+]$ or $\mathrm{M}_\Gamma[\phi]$. We again use the subroutines $\mathcal{S}_{g\gamma}$ for $g = (0, 1)$ and $\gamma \leq \Gamma$ for the operator U^+. This either determines $\mathrm{M}_\gamma[\phi^+]$ for $\gamma < \Gamma$ or determines them in terms of already known $\mathrm{M}_\Gamma[\phi^+]$.

Thus we can find either $\mathrm{M}_\gamma[\phi]$ or $\mathrm{M}_\gamma[\phi^+]$ for all $\gamma \leq \Gamma$ to estimate ϕ or ϕ^+ up to an accuracy of $2^{-\Gamma-1}$. As $\phi^+ = \phi + 2^{-\Gamma-2}$, we find ϕ up to an accuracy of $2^{-\Gamma}$. We need to apply $\mathcal{S}_{g\gamma}$ for $g = (0, 1)$ and $\gamma \leq \Gamma$, once for U and once for U^+, making a total of $4(\Gamma + 1)$ applications. If the desired accuracy in estimation of ϕ is $\delta = 2^{-\Gamma}$ then $4[\log_2 \frac{1}{\delta} + 1] = \Theta(\ln \frac{1}{\delta})$ applications of $\mathcal{S}_{g\gamma}$ are needed with 4 applications for each value of γ.

To implement $\mathcal{S}_{g\gamma}$, we choose $|\sigma\rangle = |\psi, f_\gamma\rangle$ and $\Lambda = \Lambda_{12}^{27}$ for $g = 0$ whereas $\Lambda = \Lambda_{20}^{3}$ for $g = 1$. It uses $\Theta(\ln \frac{1}{\epsilon_1})$ applications of $\mathcal{A}_{g\gamma} = R_{\psi,f'_\gamma} R_{\lambda'}$ which requires implementations of R_{ψ,f_γ} and R_λ as discussed before Eq. (5). We use our knowledge of the subspace Λ to implement R_λ. To implement R_{ψ,f_γ}, we use $|\psi, f_\gamma\rangle = \mathcal{E}(U_\gamma)|\psi\rangle|0_5\rangle$ to get $R_{\psi,f} = \mathcal{E}(U_\gamma) R_{\psi,0_5} \mathcal{E}(U_\gamma)^\dagger$ and implement $R_{\psi,0_5}$ by applying R_ψ if and only if all 5 ancilla qubits are in the $|0\rangle$ state. By definition, $\mathcal{E}(U_\gamma)$ uses $2^{5+\gamma}$ applications of U. Hence $\mathcal{A}_{g\gamma}$ needs $2^{6+\gamma}$ applications of U and 1 application of R_ψ. So $\mathcal{S}_{g\gamma}$ needs $\Theta(2^\gamma \ln \frac{1}{\epsilon_1})$ applications of U and $\Theta(\ln \frac{1}{\epsilon_1})$ applications of R_ψ where ϵ_1 is the desired error probability.

As the PEA$\approx$ uses $\Theta(\ln \frac{1}{\delta})$ applications of $\mathcal{S}_{g\gamma}$, we must choose $\epsilon_1 = \Theta(\epsilon \ln^{-1} \frac{1}{\delta})$ if ϵ is the desired error probability in the PEA$\approx$. Thus $\mathcal{S}_{g\gamma}$ uses $\Theta(2^\gamma) F_\epsilon^\delta$ and $\Theta(1) F_\epsilon^\delta$ applications of U and R_ψ respectively where F_ϵ^δ is $\ln \frac{1}{\epsilon_1} = \ln \left[\ln \frac{1}{\delta}/\epsilon\right]$. We sum these two terms from $\gamma = 0$ to $\gamma = \Gamma = \ln \frac{1}{\delta}$ to find $\mathcal{N}_\epsilon(Y)$, the total number of applications of $Y \in \{U, R_\psi\}$ needed to estimate ϕ to an accuracy of δ with the success probability $1 - \epsilon$. Thus

$$\mathcal{N}_\epsilon(U) = \Theta(\delta^{-1}) F_\epsilon^\delta, \quad \mathcal{N}_\epsilon(R_\psi) = \Theta(\ln(\delta^{-1})) F_\epsilon^\delta. \tag{21}$$

Above equation determines the time complexity of our algorithm.

Application to the BKS algorithm: We have briefly discussed the BKS algorithm in Section 2. Here $|\psi\rangle = |\theta_s\rangle$ is an approximate eigenstate of $U = V_{s+1}$ and we find θ_{s+1} up to an accuracy of $\delta = \frac{\Delta}{4}$. The BKS algorithm uses $\Theta(n)$ instances of the PEA$\approx$ and we must choose $\epsilon = \Theta(\frac{1}{n})$ for success. Thus F_ϵ^δ is $\Theta(\ln(n \ln \frac{1}{\Delta}))$. As $n > 1$ and typically $\Delta < 1$, the terms $\ln n$ and $\ln \frac{1}{\Delta}$ are $O(\ln \mathcal{Q})$ implying that $F_\epsilon^\delta = O(\ln \mathcal{Q})$ where $\mathcal{Q} = \Delta^{-1}\Theta(n \ln n)$ is the time complexity of the BKS algorithm. Also, $\Theta(n)$ instances of the PEA$\approx$ will need $\Theta(n)\mathcal{N}_\epsilon(V_s) = \frac{n}{\Delta} O(\ln \mathcal{Q})$ applications of V_s and $\Theta(n)\mathcal{N}_\epsilon(R_{\theta s}) = nO(\ln^2 \mathcal{Q})$ applications of $R_{\theta s}$ where we have used Eq. (21). As mentioned in Section 2, each $R_{\theta s}$ can be implemented using $O(\ln \frac{1}{\epsilon_0}/\Delta)$ applications of V_s and $nO(\ln^2 \mathcal{Q})$ applications of $R_{\theta s}$ are successful if we choose $\frac{1}{\epsilon_0} = \Theta(n \ln^2 \mathcal{Q})$. Then each $R_{\theta s}$ needs $\Theta(\frac{1}{\Delta}) \ln(n \ln^2 \mathcal{Q})$ applications of V_s. Thus, with our method, the number of applications of V_s used by the BKS algorithm is

$$n\Delta^{-1} O(\ln \mathcal{Q}) + \left(nO(\ln^2 \mathcal{Q}) \times \Theta\left(\Delta^{-1}\right) \ln(n \ln^2 \mathcal{Q})\right) = O(\mathcal{Q} \ln^2 \mathcal{Q}). \tag{22}$$

Though this is larger than $\mathcal{Q}$ by a logarithmic factor, we don't need multiple copies of the eigenstates which we will need if we don't use our method.

5 Discussion and Conclusion

We assumed $|\langle\psi|\phi\rangle|^2 \geq \frac{2}{3}$ only for simplicity but similar ideas can be used if $|\langle\psi|\phi\rangle|^2 \geq \frac{1}{2} + h$ for any small positive h. Then, in Eq. (15), we choose c such that $1/2(c-1)$ is h or $c \approx 1/2h$ and the lower bound in Eq. (16) becomes $(\frac{1}{2} + h)(1 - h) = \frac{1}{2} + \frac{h}{2}$. We increase μ from 5 to

$6+\log_2 h$ to get a $128c$-dimensional Hilbert space of ancilla qubits used in the PEA. Doing so also increases exponentially the required number of applications of U. Also, the subroutines $\mathcal{S}_{g\gamma}$ need to detect if $P_{g\gamma} \geq (1-h)/2$ or $P_{g\gamma} < (1+h)/2$. This increases the required number of iterations q as the error probability decreases as $e^{-qh^2/2}$ which is much larger than $e^{-q/220}$ for small h. To compensate for it, we must choose suitably large values of q. The details can be worked out easily.

An important application of the Eigenpath Traversal Problem is the quantum adiabatic evolution (QAE) where $V_s = exp(-iH_{\hat{s}}t)$ with $\hat{s} = (s-1)/(n-1)$ and $H_{\hat{s}} = (1-\hat{s})H_0 + \hat{s}H_1$ is the interpolating Hamiltonian between H_0 and H_1. It has applications to quantum computation [15]. In this case, L is $O(\|H_0 + H_1\|/\Delta)$. Childs et.al. presented an algorithm to simulate the QAE by a discrete-time quantum circuit [16] using $O(L^2/\Delta) = O(1/\Delta^3)$ time steps. The BKS algorithm can do this using $O(L/\Delta) = O(1/\Delta^2)$ time steps. The time complexity $O(1/\Delta^2)$ of the BKS algorithm is same as the evolution time $O(1/\Delta^2)$ required by the folk adiabatic approximation [7] and better than the evolution time $O(1/\Delta^3)$ required by the rigorous adiabatic approximations [17, 18, 19]. Note that the operators $V_s = e^{-iH_{\hat{s}}t}$ can be efficiently simulated for sparse Hamiltonians using recently developed simulation algorithms [20]. Recently, it was shown that if the QAE involves only the ground state then $L = O(1/\Delta^{1/2})$, much less than $O(1/\Delta)$ for $\Delta \ll 1$ [21]. Then the BKS algorithm has the time complexity $\Theta(1/\Delta^{3/2})$. Using our method, the BKS algorithm can work with just a single copy of the initial eigenstate.

We point out that in our method, the information $|\langle\psi|\phi\rangle|^2 \geq \frac{2}{3}$ is used to distinguish $|\phi\rangle$ from other eigenstates of U. Our method assumes the correctness of this information and in general, our method cannot determine whether this assumption is correct or not.

As illustrated in this paper, our method finds significant applications only in those procedures where many sequential instances of the phase estimation procedures with approximate eigenstates are needed. The Eigenpath traversal problem is one such example but other quantum algorithms may also be improved with this method and the possibilities are currently under investigation.

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