Accelerated Variational Quantum Eigensolver

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The problem of finding the ground state energy of a Hamiltonian using a quantum computer is currently solved using either the quantum phase estimation (QPE) or variational quantum eigensolver (VQE) algorithms. For precision ϵ, QPE requires $O(1)$ repetitions of circuits with depth $O(1/\epsilon)$, whereas each expectation estimation subroutine within VQE requires $O(1/\epsilon^2)$ samples from circuits with depth $O(1)$. We propose a generalized VQE algorithm that interpolates between these two regimes via a free parameter $\alpha \in [0, 1]$, which can exploit quantum coherence over a circuit depth of $O(1/\epsilon^\alpha)$ to reduce the number of samples to $O(1/\epsilon^{2(1-\alpha)})$. Along the way, we give a new routine for expectation estimation under limited quantum resources that is of independent interest.

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Introduction.—One of the most compelling uses of a quantum computer is to find approximate solutions to the Schrödinger equation. Such *ab initio* or first-principles calculations form an important part of the computational chemistry tool kit and are used to understand features of large molecules such as the active site of an enzyme in a chemical reaction or are coupled with molecular mechanics to guide the design of better drugs.

Broadly speaking, there are two approaches to *ab initio* chemistry calculations on a quantum computer: one uses the quantum phase estimation (QPE) algorithm as envisaged by Lloyd [1] and Aspuru-Guzik *et al.* [2], the other uses the variational principle, as exemplified by the variational quantum eigenvalue solver (VQE) [3]. Given a fault-tolerant device, QPE can reasonably be expected to compute energy levels of chemical species as large as the iron molybdenum cofactor (FeMoco) to chemical accuracy [4], essential to understanding biological nitrogen fixation by nitrogenase [4,5]. That QPE *may* provide a quantum-over-classical advantage can be rationalized by the exponential cost involved in naively simulating quantum gates on n qubits by matrix multiplication. One main reason that QPE requires fault tolerance is that the required coherent circuit depth, D, scales inversely in the precision ϵ. This means $D = O(1/\epsilon)$ scales exponentially in the number of bits of precision.

The VQE algorithm can also estimate the ground state energy of a chemical Hamiltonian but does so using a quantum expectation estimation subroutine together with a classical optimizer. In contrast to QPE, VQE is designed to be run on near-term noisy devices with low coherence time [3,6,7]. While VQE may also provide a quantum-over-classical advantage via the same rationalization as QPE, it suffers from requiring a large number of samples $N = O(1/\epsilon^2)$ during each expectation estimation subroutine leading to fears that its run time will quickly become unfeasible [8].

We propose a generalized VQE algorithm, we call α-VQE, capable of exploiting all available coherence time of the quantum computer to up-to-exponentially reduce the number of samples required for a given precision. The α refers to a free parameter $\alpha \in [0, 1]$ we introduce, such that for all values of $\alpha > 0$, α-VQE outperforms VQE in terms of the number of samples and has total runtime, $O(N \times D)$, reduced by a factor $O(1/\epsilon^\alpha)$. Moreover, compared to QPE, α-VQE has a lower maximum circuit depth for all $\alpha < 1$. At the two extremes, $\alpha = 0$ and $\alpha = 1$, α-VQE recovers the scaling of VQE and QPE, respectively.

The T_1 and T_2 coherence times of the quantum computer essentially define a maximum circuit depth, $D_{\max}$, that can be run with a low expected number of errors [9]. By choosing an $\alpha \in [0, 1]$ such that the maximum coherent circuit depth $D(\alpha) = O(1/\epsilon^\alpha)$ of the expectation estimation subroutine in α-VQE equals $D_{\max}$, we show that the expected number of measurements N required can be reduced to $N = f(\epsilon, \alpha)$, where

$$f(\epsilon,\alpha) = \begin{cases} \dfrac{2}{1-\alpha}\left(\dfrac{1}{\epsilon^{2(1-\alpha)}} - 1\right) & \text{if } \alpha \in [0,1) \\ 4\log\left(\dfrac{1}{\epsilon}\right) & \text{if } \alpha = 1 \end{cases}. \quad (1)$$

Note that $f(\epsilon, 0) = O(1/\epsilon^2)$ is proportional to the number of measurements taken in VQE, whereas $f(\epsilon, 1) = O(\log(1/\epsilon))$ is the number of measurements taken in iterative QPE up to further log factors.

Our letter is organized as follows. We generalize VQE to α-VQE by replacing its expectation estimation subroutine with a tunable version of QPE we name α-QPE. This is set out in three steps. First, we introduce $\alpha \in [0, 1]$ into a Bayesian QPE [10] to yield α-QPE. Second, we describe how to replace the expectation estimation subroutine within

VQE by α-QPE by modifying a result of Knill *et al.* [11]. Third, we give a schematic illustration of the resulting α-VQE. We conclude our letter by explaining how α-VQE accelerates VQE.

Generalizing VQE to α-VQE.—The standard VQE algorithm is inspired by the use of variational ansatz wave functions $|\psi(\lambda)\rangle$, depending on a real vector parameter λ, in classical quantum chemistry. The ground state energy of a Hamiltonian H is found by using a hybrid quantum-classical computer to calculate the energy $E(\lambda)$ of the system in the state $|\psi(\lambda)\rangle$, and a classical optimizer to minimize $E(\lambda)$ over λ.

The idea is to first write H as the finite sum $H = \sum a_i P_i$, where a_i are real coefficients and P_i are a tensor product of Pauli matrices. The number of summed terms is typically polynomial in the system size, as is the case for the electronic Hamiltonian of quantum chemistry. Then for a given (normalized) $|\psi(\lambda)\rangle$ we estimate the energy,

$$E(\lambda) \equiv \langle\psi(\lambda)|H|\psi(\lambda)\rangle = \sum_i a_i \langle\psi(\lambda)|P_i|\psi(\lambda)\rangle, \quad (2)$$

using a quantum computer for the individual expectation values and a classical computer for the weighted sum. Finally a classical optimizer is used to optimize the function $E(\lambda)$ with respect to λ by controlling a preparation circuit $R(\lambda): |0\rangle \mapsto |\psi(\lambda)\rangle$ where $|0\rangle$ is some fixed starting state. The variational principle justifies the entire VQE procedure: writing $E_{\min}$ for the ground state eigenvalue of H, we have that $E(\lambda) \geq E_{\min}$ with equality if and only if $|\psi(\lambda)\rangle$ is the ground state.

Each expectation $\langle\psi(\lambda)|P_i|\psi(\lambda)\rangle$ is directly estimated using statistical sampling [12]. The circuit used has extra depth $D = O(1)$ beyond preparing $|\psi(\lambda)\rangle$ and is repeated $N = O(1/\epsilon^2)$ times to attain precision within ϵ of the expectation. Henceforth, we refer to this N, D scaling with ϵ as the statistical sampling regime.

Tunable Bayesian QPE (α-*QPE*): Since the introduction by Kitaev [13] of a type of iterative QPE involving a single work qubit and an increasing number of controlled unitaries following each measurement, the term QPE itself has become associated with algorithms of this particular type. It is characteristic of Kitaev-type algorithms that for precision ϵ, the number of measurements $N = \tilde{O}(\log(1/\epsilon))$ and maximum coherent depth $D = \tilde{O}(1/\epsilon)$, where the tilde means we neglect further log factors. Henceforth, we refer to this N, D scaling with ϵ as the phase estimation regime and QPE as phase estimation in this regime.

For a given eigenvector $|\phi\rangle$ of a unitary operator U such that $U|\phi\rangle = e^{i\phi}|\phi\rangle$, $\phi \in [-\pi, \pi)$, Kitaev's QPE algorithm uses the circuit in Fig. 1 with two settings of $M\theta \in \{0, -\pi/2\}$. For each setting, $N = \tilde{O}(\log(1/\epsilon))$ measurements are taken with $M = 2^{m-1}, 2^{m-2}, \ldots, 1$ in that order to estimate ϕ to precision $\epsilon \equiv 2^{-m}$. In Kitaev's algorithm, "precision ϵ" means "within error ϵ above a constant level of probability." The coherent circuit depth D required is therefore

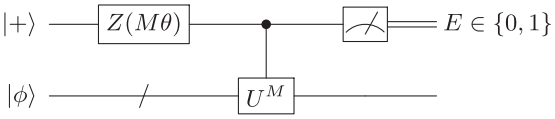

FIG. 1. Circuit for Kitaev's phase estimation and RFPE. Here, $|\phi\rangle$ is an eigenstate of U with eigenphase ϕ, $|+\rangle$ is the $+1$ eigenstate of X, $Z(M\theta) \coloneqq \mathrm{diag}(1, e^{-iM\theta})$, and measurement is performed in the X basis.

$$D = \tilde{O}\left(\sum_{j=0}^{m-1} 2^j\right) = \tilde{O}(2^m) = \tilde{O}(1/\epsilon). \quad (3)$$

This accounting associates to U^{2^j} a circuit depth of $O(2^j)$. For generic $U = \exp(-iHt)$, any better accounting is prohibited by the "no-fast-forwarding" theorem [14]. We do not consider special U such that U^{2^j} has better accounting (e.g., modular multiplication in Shor's algorithm [15]).

Under the framework of Kitaev's QPE, Wiebe and Granade [10,16] introduced a Bayesian QPE named rejection filtering phase estimation (RFPE) that we now modify to yield different sets of circuit and measurement sequences that can provide the same precision ϵ with different (N, D) trade-offs. It is these sets that are parametrized by the $\alpha \in [0, 1]$. The circuit for RFPE is given in Fig. 1 and the following presentation of RFPE and our modification is broadly self-contained.

To begin, a prior probability distribution $P(\phi)$ of ϕ is taken to be normal $\mathcal{N}(\mu, \sigma^2)$ (some justification is given in Ref. [17], which empirically found that the posterior of a uniform prior converges rapidly to normal). From the RFPE circuit in Fig. 1, we deduce that the probability of measuring $E \in \{0, 1\}$ is

$$P(E|\phi; M, \theta) = \frac{1 + (-1)^E \cos[M(\phi - \theta)]}{2}, \quad (4)$$

which enters the posterior by the Bayesian update rule,

$$P(\phi|E; M, \theta) \propto P(E|\phi; M, \theta) P(\phi). \quad (5)$$

We do not need to know the constant of proportionality to sample from this posterior after measuring E, and the word rejection in RFPE refers to the rejection sampling method used. After obtaining a number s of samples, we approximate the posterior again by a normal with mean and standard deviation equal to that of our samples (again

justified as when taking initial prior to be normal). The choice of s is important and s can be regarded as a particle filter number, hence the word filter in RFPE [16]. We constrain posteriors to be normal because normal distributions can be efficiently sampled.

The effectiveness of RFPE's iterative update procedure just described depends on controllable parameters (M, θ). A natural measure of effectiveness is the expected posterior variance, i.e., the "Bayes risk." To minimize the Bayes risk, Ref. [10] chooses $M = \lceil 1.25/\sigma \rceil$ at the start of each iteration. However, the main problem is that M can quickly become large, making the depth of U^M exceed $D_{\max}$. Reference [16] addresses this problem by imposing an upper bound on M and we refer to this approach as RFPE with restarts.

Here, we propose another approach that chooses

$$(M, \theta) = \left(\frac{1}{\sigma^\alpha}, \mu - \sigma\right), \tag{6}$$

where $\alpha \in [0, 1]$ is a free parameter we impose. Moreover, we propose a new preparation of eigenstate $|\phi\rangle$ at each iteration, discarding that used in the previous iteration. This ability to readily prepare an eigenstate is highly typical but can be achieved within the VQE framework (see next section). We name the resulting, modified RFPE algorithm α-QPE. In proposition 1 below, we give the main performance result about α-QPE. We defer its derivation to Supplemental Material [18]. Unlike in Kitaev's algorithm, we henceforth let precision ϵ mean an expected posterior standard deviation of ϵ [21].

Proposition 1. (Measurement-depth trade-off). For precision ϵ, α-QPE requires $N = f(\epsilon, \alpha)$ measurements and $D = O(1/\epsilon^\alpha)$ coherent depth, where the function f is defined in Eq. (1).

We now address the essential question of how to choose α when practically constrained to circuits with bounded depth $D \in [1, D_{\max}]$ for some $D_{\max}$. For simplicity, we assume $D = 1/\epsilon^\alpha$. Optimally choosing α amounts to minimizing the number of measurements N to achieve a fixed precision $\epsilon \in (0, 1)$. Then, because $N = f(\epsilon, \alpha)$ is a decreasing function of α, the least N is attained at the maximal $\alpha = \alpha_{\max} := \min\{[\log(D_{\max})]/[\log(1/\epsilon)], 1\}$, giving $N_{\min} = f(\epsilon, \alpha_{\max})$, which equals

$$\begin{cases} \frac{2}{1-\log(D_{\max})/\log(1/\epsilon)}\left[\left(\frac{1}{\epsilon D_{\max}}\right)^2 - 1\right] & \text{if } D_{\max} < \frac{1}{\epsilon} \\ 4\log\left(\frac{1}{\epsilon}\right) & \text{if } D_{\max} \geq \frac{1}{\epsilon} \end{cases}. \tag{7}$$

The important point here is the inverse quadratic scaling with $D_{\max}$ if $D_{\max} < 1/\epsilon$: through α we can access and exploit $D_{\max}$ to significantly reduce the number of iterations. In Supplemental Material [18], we deduce from our above analysis that RFPE is at least as efficient as Eq. (7).

Casting expectation estimation as α-QPE: Given a Pauli operator P, a preparation circuit $R(\lambda) \equiv R: |0\rangle \mapsto |\psi(\lambda)\rangle \equiv |\psi\rangle$, and a projector $\Pi := I - 2|0\rangle\langle 0|$, we paraphrase from Knill *et al.* [11] the following proposition 2 relevant to us.

Proposition 2. (Amplitude estimation). The operator $U := U_0 U_1$, with $U_0 = (R\Pi R^\dagger)$, $U_1 = (PR\Pi R^\dagger P^\dagger)$, is a rotation by an angle $\phi = 2\arccos(|\langle\psi|P|\psi\rangle|)$ in the plane spanned by $|\psi\rangle$ and $|\psi'\rangle := P|\psi\rangle$. Therefore, the state $|\psi\rangle$ is an equal superposition of eigenstates $|\pm\phi\rangle$ of U with eigenvalues $e^{\pm i\phi}$, respectively (i.e., eigenphases $\pm\phi$) and we can estimate $|\langle\psi|P|\psi\rangle| = \cos(\pm\phi/2)$ to precision ϵ by running QPE on $|\psi\rangle$ to precision 2ϵ.

Note that the VQE framework readily provides $R(\lambda)$, which enables our use of proposition 2. We now modify proposition 2 to use α-QPE, which enables access to the measurement-depth trade-off given in proposition 1. Since α-QPE requires repreparation of state $|\pm\phi\rangle$ at each iteration, a complication arises because $|\psi\rangle$ is in equal superposition of $|\pm\phi\rangle$. To be able to efficiently collapse $|\psi\rangle$ into one of $|\pm\phi\rangle$ with high confidence before each iteration in α-QPE, we have to assume that $|A|$ is always bounded away from 0 and 1 by a constant $\delta > 0$, where $A = \langle\psi|P|\psi\rangle$ (see Ref. [11] [parallelizability]). If we collapse into $|\phi\rangle$ (with high confidence), we implement α-QPE using (powers of) c-U; or else if we collapse into $|-\phi\rangle$, we use c-$U^\dagger$. The depth overhead of state collapse is $O(1/\delta)$. A second complication is that ϕ gives $|A|$ but not the sign of A.

These two complications can be simultaneously resolved using a simple two-stage method. In the first stage, A is roughly estimated by statistical sampling a constant number of times to determine whether $|A|$ satisfies a δ bound. If so, proceed with α-QPE, or else continue with statistical sampling in the second stage. The first stage simultaneously determines the sign of A. In Supplemental Material [18], we present further details of this method.

The overhead in implementing c-$U = R(c\text{-}\Pi)R^\dagger PR(c\text{-}\Pi)R^\dagger P$ is documented as follows. Since P is n tensored Pauli matrices, it can be implemented using n parallel Pauli gates in $O(1)$ depth. The $(n+1)$-qubit controlled sign flip c-Π is equivalent in cost, up to $\sim 2n$ single qubit gates with $O(1)$ depth, to an $(n+1)$-bit Toffoli gate, the best-known implementation of which requires $6n - 6$ CNOT gates [22], $\lceil (n-2)/2 \rceil$ ancillas, and $O(\log n)$ circuit depth [23]. Lastly, we need two R and two $R^\dagger \equiv R^{-1}$. Since the depth C_R of R is $\Omega(n)$ in most applications considered so far [24], this last overhead may be the most significant. As the total overhead has no ϵ dependence, it does not affect our analysis in terms of ϵ.

Generalized α-VQE: We define generalized α-VQE as VQE but with its expectation estimation subroutines cast as α-QPE in the manner above. Figure 2 illustrates the schematic of our generalized VQE.

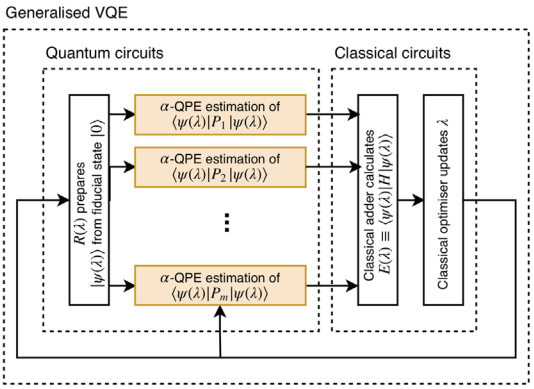

FIG. 2. Schematic of α-VQE. Note that λ also affects α-QPE circuits, which involve state preparation $R(\lambda)$ and its inverse. When $\alpha = 0$, we are in the statistical sampling, or standard VQE, regime. When $\alpha = 1$, we are in the phase estimation regime.

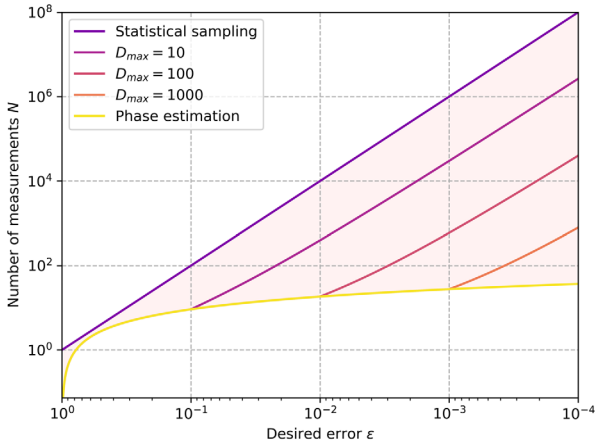

FIG. 3. Plots of the function in Eq. (7) for different $D_{\max}$ demonstrate how α-VQE accelerates VQE by reducing the number of measurements up to exponentially as $D_{\max}$ increases. Also plotted are the statistical sampling and phase estimation regimes. α-VQE unlocks regimes in the shaded region between these two extremes.

The total number of measurements in an entire run of α-VQE is of order $f(\epsilon, \alpha)$ multiplied by both the number of summed terms in the Hamiltonian and the number of iterations of the classical optimizer. Writing C_R for the depth of $R(\lambda)$, each measurement results from a circuit of depth $O((C_R + \log n)/\epsilon^{\alpha})$.

Clearly, α-VQE still preserves the following three key advantages of standard VQE because we only modified the expectation estimation subroutine. First, we can parallelize the expectation estimation of multiple Pauli terms to multiple processors. Second, robustness via self-correction is preserved because α-VQE is still variational [6,7]. Third, the variational parameter λ can be classically stored to enable straightforward repreparation of $|\psi(\lambda)\rangle$ [8].

α-VQE as accelarated VQE.—We reiterate that α-VQE is useful because it can perform expectation estimation in regimes lying continuously between statistical sampling and phase estimation. Neither extreme is ideal: statistical sampling requires $N = O(1/\epsilon^2)$ samples whereas phase estimation requires $D = O(1/\epsilon)$ coherence time. In this manner, these two extremes have been criticised in Ref. [25] and Refs. [3,6], respectively, and compared in Ref. [8].

The resources required for one run of expectation estimation within VQE and α-VQE (arbitrary α, $\alpha = 0$, $\alpha = 1$) are compared in Table I. Neglecting the small overheads to cast expectation estimation as α-QPE, we can conclude that our method of expectation estimation is always superior to statistical sampling for $\alpha > 0$.

To use $\alpha > 0$, we need sufficiently large $D_{\max}$. Conversely, given $D_{\max}$ we can choose an α to maximally exploit it. Doing so yields the acceleration quantified by Eq. [7]. This provides the mechanism by which α-VQE accelerates VQE. The acceleration is quantified by Eq. (7). We plot Eq. (7) in Fig. 3 to give a concrete sense of our contribution.

At a more theoretical level, we note that our letter can be viewed outside the VQE context as a study of efficient expectation estimation under restricted circuit depth. Furthermore, our study of α-QPE can be viewed as a study of phase estimation under restricted circuit depth. Subsequently to our letter, Ref. [26] also studied this latter question, proposing and analyzing a time series estimator that learns the phase with similar efficiency as our results. More precisely, their efficiency Eq. (22) conforms to our Eq. (7) up to log factors.

TABLE I. Resource comparison of one expectation estimation subroutine within VQE, 0-VQE, 1-VQE, α-VQE. ϵ is the precision required for the expected energy, C_R is the state preparation depth, and $\alpha \in [0, 1]$ is the free parameter controlling the maximum circuit depth of α-QPE.

Algorithm	Maximum coherent depth	Noncoherent repetitions	Total runtime
VQE	$O(C_R)$	$O(1/\epsilon^2)$	$O[C_R(1/\epsilon^2)]$
0-VQE	$O(C_R + \log n)$	$O(1/\epsilon^2)$	$O((C_R + \log n)(1/\epsilon^2))$
1-VQE	$O((C_R + \log n)(1/\epsilon))$	$O[\log(1/\epsilon)]$	$O((C_R + \log n)(1/\epsilon))$
α-VQE	$O((C_R + \log n)(1/\epsilon^{\alpha}))$	$O(f(\epsilon, \alpha))$	$O((C_R + \log n)(1/\epsilon^{\alpha}) f(\epsilon, \alpha))$

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