Variational Quantum Eigensolvers: An Overview

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Abstract

In this paper we study the variational quantum eigensolver algorithm, a method for estimating the ground state energy of a many-body Hamiltonian. A broad overview of the protocol is presented, discussing the mathematical theory, as well as the motivations from quantum chemistry. Three of the first experimental implementations of the algorithm are presented, along with an extension of the algorithm which gives the protocol the ability to estimate excited state energies, in addition to the ground state.

1 Introduction

One of the most fundamental goals in quantum chemistry is to be able to determine the ground state of a Hamiltonian which describes an atom or molecule. From a classical computing perspective, we may attempt to solve this problem, given a Hamiltonian, by representing the operator as a matrix and using standard linear algebra techniques to find its eigenvalues and eigenvectors. However, as the size of the matrix increases exponentially with the number of particles in the system, this technique becomes infeasible for all but the smallest atoms and molecules.

One of the first steps to tackle this problem using quantum computing was designed by Alexei Kitaev in 1995 [1]. His *Quantum Phase Estimation* (QPE) algorithm allows the efficient computation of the eigenvalues of any unitary operator that is implemented as a quantum gate in a quantum circuit. In order to estimate the eigenvalues of a given Hamiltonian, H, using QPE, a unitary matrix is constructed, by taking the exponential e^{-iH}. Once the eigenvalues of this matrix are known, the eigenvalues of H are simply the natural logarithm (with a factor of i) of the eigenvalues of the unitary matrix. Unfortunately, in order to compute this matrix exponential exactly, we need to already know the eigenvalues of the Hermitian matrix, H. Thus is appears that QPE may not be helpful for our quantum chemistry problem after all. Luckily, there exist techniques which may be used to approximate matrix exponentials, such as the Trotter-Suzuki approximation [2], which decomposes H into a sum of matrices whose exponentials are either simple to compute, or already well known.

However, even after obtaining a form of the Hamiltonian on which we may perform QPE to find the ground state, this algorithm suffers from other problems related to precision and circuit depth. In order to obtain an accurate result from QPE within an environment which induces small perturbations to the quantum computer, each step in the computation must be performed with some precision, ϵ, which depends on the allowed error probability of the computation. Furthermore, it is known that achieving a precision ϵ in QPE requires a circuit depth of order $O(1/\epsilon)$. Note that the term *precision* here essentially refers to the least significant digit of the quantity under inspection, and is thus much less than one for very precise values. To put this into a more illustrative form, we may transform the precision into the number of *precision bits*, using exponentiation. For example, if we require 2 precision bits, that means that we need an accuracy to the hundredths, which is a precision of $\epsilon = 0.01$. It is easy to see that $\epsilon = 10^{-2}$, and in general, $\epsilon = 10^{-b}$, gives the precision ϵ, in terms of the number of precision bits, b. In that case, we have the circuit depth must be $O(1/\epsilon) = O(1/10^{-b}) = O(10^{b})$. So the circuit depth must actually be exponential in the number of precision bits. This is very troublesome, as the circuit depth quantifies how long the qubits in the quantum computer must stay coherent. Presently, maintaining quantum coherence for extended periods of time remains a difficult and central problem to the field of quantum information.

One method to mitigate this issue, is to introduce fault tolerance into the quantum circuit. This reduces the effects of small perturbations on the system, reducing the number of precision bits necessary for each step in the computation to remain above a chosen error threshold, and thus reduces the required circuit depth. However, we may also choose to set aside the QPE algorithm, in favour of another. Instead of looking to fault tolerance to improve QPE, Peruzzo et al. considered an alternative method for determining the ground state of a given Hamiltonian, known as *variational quantum eigensolvers* (VQE) [3]. This algorithm is based on the *variational method* and trades a short quantum circuit depth for a large number of iterations. More specifically, the VQE algorithm achieves a precision ϵ with a circuit depth $O(1)$ and a number of iterations $O(1/\epsilon^2)$. Using our previous transformation from precision to number of precision bits, we see that the number of iterations necessary for VQE scales exponentially in the number of precision bits, while the circuit depth is constant. This trade-off is quite appealing for experimentalists, as it currently much easier (if time consuming) to repeatedly run an algorithm, than it is to maintain quantum coherence for extended periods of time.

In this paper we shall explore the VQE algorithm with the intent to not only understand the mathematical theory and scientific motivation behind it, but also to see its experimental implementations and get an idea of how to extend the algorithm to incorporate other useful capabilities. In Section 2 we discuss the underlying theory involved in VQE. We examine the mathematical underpinnings, as well as its motivations in computational and quantum chemistry. Section 3 introduces three of the first experimental implementations of VQE, which use photonic qubits, ion trap qubits, and superconducting qubits, respectively, for their quantum processing. Finally, in Section 4 we discuss one of the ways in which the VQE algorithm may be extended, to compute excited states as well as the ground state of a given Hamiltonian.

2 Theory

2.1 The Variational Method

Our study of the VQE algorithm begins with a discussion of the *Rayleigh quotient.* This quotient is defined for Hermitian matrices as follows:

$$R(H, x) \equiv \frac{x^\dagger H x}{x^\dagger x}.$$

The Rayleigh quotient is extremely useful in determining the eigenvalues of a Hermitian matrix, through the use of the *min-max theorem*:

Theorem 1 *Let H be an $n \times n$ Hermitian matrix and let x be a vector in $\mathbb{C}^n$. Order the eigenvalues of H as $\lambda_1 \geq \ldots \geq \lambda_n$. Then we have the following relationships:*

$$\lambda_k = \max_V \{ \min_x \{ R(H, x) | x \in V \mathit{and}\ x \neq 0 \} | \dim(V) = k \}$$

and

$$\lambda_k = \min_V \{ \max_x \{ R(H, x) | x \in V \mathit{and}\ x \neq 0 \} | \dim(V) = n - k + 1 \},$$

where V is a subspace of $\mathbb{C}^n$.

In particular, if we consider the smallest eigenvalue, λ_n, we may use the first expression for λ_k, noting that there is only one subspace of $\mathbb{C}^n$ with dimension n, and that is $\mathbb{C}^n$ itself. Thus we have

$$\lambda_1 = \min_{x\in\mathbb{C}^n, x\neq 0} R(H, x).$$

Moreover, it can be shown that when attempting to minimize the Rayleigh quotient with non-zero x, it is sufficient to consider normalized x. Thus the Rayleigh quotient reduces to $x^\dagger H x$ - i.e. we simply compute the expectation value of H with respect to x. Thus we may attempt to find the smallest eigenvalue of H by repeatedly computing the expectation value of H with respect to a vector $x(\theta)$, which depends on some parameters θ, and tuning the parameters, until we minimize the expectation value. This idea is known as the *variational principle* - it is possible to compute the extreme values of some quantities by finding extreme values of some other function on which those quantities depend. This simple idea, and in particular the min-max theorem, is the backbone of the VQE algorithm: if we can minimize the expectation value of a given Hamiltonian, then we can find its ground state.

With this in mind, we are now prepared to explore VQE proper. We begin by noting that we may expand any Hermitian operator as a linear combination of tensor products of Pauli operators (i.e. elements of the Pauli group). For concreteness, let us write a Hamiltonian, H, as:

$$H = \sum_{P_i\in\mathcal{P}} h_i P_i,$$

where $\mathcal{P}$ is the Pauli group, P_i are Pauli group elements, and we allow some of the coefficients, h_i, to be 0.

Then determining the expectation value of H is equivalent to computing the expectation values of each of the Pauli group elements P_i (with $h_i \neq 0$), and then performing a weighted sum.

While quantum computers may outperform their classical counterparts in many tasks, classical computation is completely sufficient for efficiently computing summations. In contrast, there exists a quantum circuit which out-performs all classical algorithms when computing the expectation values of a tensor product of Pauli matrices [4]. We can then see that the basic mechanics of VQE (computing expectation values and weighted sums) may be performed by a combination of classical and quantum computing. Furthermore, having the opportunity to share the computational load between classical and quantum computing elements in VQE, suggests a type of efficiency may be found in this algorithm which cannot be achieved in QPE (which uses purely quantum computing elements). In particular, this hybrid-computing style is very effective at reducing the required coherence times of qubits, as coherence is only necessary during quantum processing.

We have now reduced the problem of finding the expectation value of a given Hamiltonian, to two simpler problems: finding expectation values of Pauli group elements, and addition. However, we must be mindful of a subtle point: we can only use this procedure on Hamiltonians with a number of Pauli terms which scales polynomially in the size of the system. Hamiltonians with exponentially many Pauli terms cannot be efficiently processed, even with a quantum computer. However, this restriction is not a significant limitation, as the set of Hamiltonians with a polynomial number of Pauli terms is quite vast, including the electronic structure Hamiltonian of quantum chemistry, the quantum Ising model, and the Heisenberg model [5], as well as those matrices which are well approximated by a sum of n-fold tensor products [6].

With the basic idea behind the VQE algorithm in mind, we next turn to the question of how to choose the vectors which will be used to compute the expectation values of the Pauli operators. In order to build an intuition behind our choice of vectors, we will begin by motivating our choice using ideas from quantum and computational chemistry.

2.2 Slater Determinant and Permanent

Long before either of the VQE or QPE algorithms were presented, chemists had been hard at work, approximating the ground states atoms and molecules using purely classical means. One of the main tools of computational chemistry is known as the *Hartee-Fock method.* This method guesses that the ground state wave function of a many-body system has a particular form, given by a *Slater determinant* in the case of a system of fermions, and a *permanent* in the case of bosons. This idea will prove to be applicable to the VQE algorithm as well, and so we shall begin our journey into the field of computational chemistry by considering the ideas of the Slater determinant and permanent.

It is well-known that any wave function describing a system of two indistinguishable fermions, $\psi(x_1, x_2)$ must be antisymmetric under the exchange of its two indices: $\psi(x_1, x_2) = -\psi(x_2, x_1)$. Given wave functions for two individual particles, $\phi_1(x_1)$ and $\phi_2(x_2)$, it is natural to try to define a wave function for the composite system as simply the product $\phi_1(x_1)\phi_2(x_2)$. However this is clearly not antisymmetric (or even symmetric) under the exchange of the indices x_1 and x_2. Thus this is not an appropriate wave function for fermions (or bosons). Still, it is simple to construct an appropriate wave function for a system of two indistinguishable fermions using

$\phi_1(x_1)$ and $\phi_2(x_2)$:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1)].$$

This wave function is antisymmetric under the exchange of its indices. But, perhaps more intriguingly, it may be written as a determinant:

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \phi_1(x_1) & \phi_2(x_1) \\ \phi_1(x_2) & \phi_2(x_2) \end{vmatrix}$$

What John C. Slater told us, is that we may generalize this wave function to a system of N identical fermions by simply constructing the determinant of a larger matrix, with entries made up of all of the possible combinations of single-fermion wave functions ϕ_j and indices x_i, and attaching an appropriate normalization factor:

$$\psi(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(x_1) & \phi_2(x_1) & \ldots & \phi_N(x_1) \\ \phi_1(x_2) & \phi_2(x_2) & \ldots & \phi_N(x_2) \\ \vdots & \vdots & \ldots & \vdots \\ \phi_1(x_N) & \phi_2(x_N)\ldots & \phi_N(x_N) \end{vmatrix}$$

Wave functions of this form are known as *Slater determinants*. It is easy to see that wave functions of this form are antisymmetric under the exchange of any two indices: exchanging indices x_i and x_j causes the ith and jth rows of the matrix to be swapped, and the determinant of any matrix picks up a phase of -1 under the exchange of any two of its rows.

In the case of bosons, we demand the wave function to be symmetric under the exchange of any two indices. The Slater determinant method is easily extended to the case of bosons, by performing the operation of the *permanent* on the same matrix as defined above. The permanent operation is the same as the determinant operation, except all of the subtractions are turned into addition. For example, the 3 × 3 case gives us the following permanent:

$$\text{perm}(\begin{bmatrix} a & b & c \\ e & f & g \\ h & i & j \end{bmatrix}) = afj + aig + bej + bgh + cei + cfh$$

We can then see that in the 2 × 2 case, forming the same matrix as for the Slater determinant, but invoking the permanent instead of the determinant, will give us the wave function

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}}[\phi_1(x_1)\phi_2(x_2) + \phi_1(x_2)\phi_2(x_1)].$$

Furthermore, it turns out that permanent of any matrix is unchanged under the exchange of any two rows, and thus permanent wave functions will be symmetric under the exchange of any two indices x_i and x_j, and so are appropriate wave functions for systems of bosons.

We previously mentioned that in order to perform VQE, we need to take the expectation value of H with respect to some parameterized vector, $x(\theta)$. By finding appropriate parameters θ to minimize the expectation value, we determine the ground state energy. The optimal parameters can be found using a classical minimization algorithm, such as gradient descent [7]. We shall next consider how to find such a parameterized vector, which we shall call the *ansatz* wave function, and the corresponding parameters. We should first note, that we cannot permit ourselves to have exponentially many parameters characterizing our state (that is, exponential in the size of our system), in much the same way that we could not have exponentially many Pauli terms in our Hamiltonian decomposition - such states would not be efficiently preparable, even by a quantum computer. Thankfully, once again, this is not much of a limitation.

It may not be too surprising to find out that the Slater determinant and permanent wave functions will be very useful in constructing our ansatz. As previously mentioned, Slater determinant and permanent wave functions are assumed to be the exact ground state wave functions of atoms or molecules when using the Hartree-Fock method. We shall refer to these states as *Hartree-Fock ground states.* Similar to the VQE algorithm, the Hartee-Fock method invokes the variational principle in order to compute the ground state energy of a given atom or molecule. The main difference between these two procedures (besides the fact that the VQE algorithm is specifically designed to take advantage of quantum processors and their abilities to compute expectation values Pauli group elements efficiently) comes from the choice of ansatz wave function. While the Hartree-Fock method first guesses the ground state wave function to be a Hatree-Fock ground state, and then uses the variational method to tune this choice to a more accurate wave function, the VQE algorithm begins by considering the *unitary coupled cluster ansatz* (UCCA).

2.3 Coupled Cluster Ansatz

The non-unitary form of the UCCA, simply called the coupled cluster ansatz (CCA), has been a powerful tool in quantum chemistry since its introduction to the field in 1966 [8]. It has been used so extensively and to such great effect, in fact, that it has been dubbed the “gold standard of quantum chemistry” [9]. The CCA takes the form

$$|\Psi\rangle = e^T |\Phi\rangle_{ref},$$

where T is the so-called *cluster operator*, and $|\Phi\rangle_{ref}$ is a *reference state*. This reference state is generally taken to be the Hartree-Fock ground state of the atom or molecule under consideration.

The cluster operator T, has the form $T = T_1 + \ldots + T_N$, for an N particle system. Each of the T_i, in turn, are summations of *excitation operators* (extremely important operators in the second quantization formalism):

$$T_1 = \sum_{pr} t_p^r a_p^\dagger a_r,$$

$$T_2 = \sum_{pqrs} t_{pq}^{rs} a_p^\dagger a_q^\dagger a_r a_s$$

and so on. Operators of the form $a_p^\dagger a_r$ are known as *single excitation operators*, $a_p^\dagger a_q^\dagger a_r a_s$, are *double excitation operators*, and so forth. The t's are simply coefficients. We shall see these excitation operators again shortly, as the language of second quantization is all but required for the study of many-body systems.

While the non-unitary coupled cluster ansatz is used to estimate the ground state energy of a molecular system, this estimate is not performed in same manner as in VQE (or the Hartree-Fock method). In particular, the energy estimation comes in the form of a *generalized expectation value*, $E = \langle (1 + \Lambda) e^{-t} H E^T \rangle$, where Λ is *de-excitation operator*. Coupled cluster theory is a vast topic, requiring a strong background in second quantization, and its complete formalism is outside of the scope of this paper. More can be found on the theory, including the appearance and properties of the de-excitation operator, Λ, in these resources [10, 11, 12]. For our present purposes, we will not be too concerned with the form of the generalized expectation value, other than to say that it is known to be sufficiently adept at estimating the ground state energy of a Hamiltonian, and even comes with its own set of benefits. Chief amongst these benefits is *size-extensivity* - that is, this method of computing ground state energies produces energies which scale appropriately with the size of the investigated system [13]. The property of size-extensivity, introduced by Bartlett [14], is an important consideration when constructing new methods for estimating energies in many-body systems, as it assures us that we do not need to worry about our method breaking down when the size of our system gets too large.

However, the CCA also has the unfortunate drawback of not providing a *variational bound* on the ground state energy. Recall that when computing (non-generalized) expectation values of a Hamiltonian, each expectation value provides an upper bound on the true ground state energy. This is not the case for the generalized expectation value. In cases where the CCA is not an appropriate estimate of the ground state wave function, the energy determined by this ansatz may diverge toward negative infinity. One example of this behaviour was found when studying the N_2 bond-breaking curve [15]. To circumvent this issue, a unitary modification of the coupled-cluster ansatz was introduced: replace T in the non-unitary ansatz with $T - T^\dagger$, to receive the unitary coupled cluster ansatz. The energy found using the UCCA turns out to be simply the expectation value of the Hamiltonian with respect to this ansatz. This means (due to the min-max theorem) that the UCCA *does*, in fact, produce a variational bound on the ground state energy (so we do not have to worry about negative infinity divergences). Moreover, the UCCA method is also size-extensive [16].

As the operator $e^{T-T^\dagger}$ is unitary, we may interpret the UCCA, $e^{T-T^\dagger} \left|\Phi\right\rangle_{ref}$ as a time evolved Hartree-Fock ground state under the Hamiltonian $i\hbar(T - T^\dagger)$. With this in mind, it is possible to efficiently create a UCCA using a quantum circuit [4]. As the UCCA is used as the parameterized vector in VQE, we should note that the parameterization refers to the t coefficients of the ansatz. By appropriately tuning these coefficients, we aim to minimize the expectation value of a given Hamiltonian with respect to the UCCA.

We now have nearly every piece required for VQE: we know the mathematical motivation of our algorithm, we understand our procedure for computing expectation values, we know what our states look like, but we have neglected one question: We know that we can write out any Hamiltonian as a weighted sum of Pauli group elements, but how do we do this?

2.4 Decomposing the Hamiltonian

We need a prescription for decomposing a Hamiltonian into a weighted sum of Pauli group elements. Such a method begins by applying the *Born-Oppenheimer approximation* to the system being analyzed. This approximation states that the total wave function of a molecular system may be written separably as the tensor product of a nuclear wave function and a electronic wave function: $\Psi_{tot} = \psi_{nuclear} \otimes \psi_{electronic}$. For our purposes, it is more important to consider this assumption in terms of the Hamiltonian: our molecular Hamiltonian will be separable, of the form $H = H_{nuclear} \otimes H_{electronic}$. We note that the eigenvalues of a tensor product of operators are simply the products of the eigenvalues of the individual operators. Thus, with the above assumption, we have that the ground state energy of our molecular Hamiltonian will be the product of the ground state energies of $H_{nuclear}$

and $H_{electronic}$. Furthermore, the Born-Oppenheimer approximation also assumes that the kinetic energy of the nuclei in the investigated molecule may be neglected. With this assumption in place, it is generally much easier to study the nuclear Hamiltonian than the electronic one. In fact, it is often assumed that the ground state energy of a nuclear Hamiltonian is known, and techniques such as the Hartree-Fock method, the CCA and UCCA methods, and even VQE, are only applied to the electronic Hamiltonian of a system. We will make this assumption as well. So from now on, we will only be considering electronic Hamiltonians.

With the Born-Oppenheimer approximation in place, it is known that the (electronic) Hamiltonian of a molecular system may be written, using second quantization, as [17]:

$$H = \sum_{pq} h_{pq}(R)\hat{a}_p^\dagger \hat{a}_q + \sum_{pqrs} h_{pqrs}\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s,$$

where R characterizes the positions of the nuclei in the system, and

$$h_{pq}(R) = \int dr\phi_p^*(r)(-\frac{1}{2}\nabla^2 - \sum_\alpha \frac{Z_\alpha}{|R_\alpha - r|})\phi_q(r)$$

and

$$h_{pqrs} = \int dr_1 dr_2 \frac{\phi_p^*(r_1)\phi_q^*(r_2)\phi_r(r_1)\phi_s(r_2)}{|r_1 - r_2|}.$$

Note that the $\phi(r)$ refer to single electron wave functions, Z_α is the nuclear charge of the αth atom in the system, and R_α is the position of the αth atom.

We note the familiar single and double excitation operators in the first and second sums of the Hamiltonian (a hallmark of second quantization). Furthermore, the forms of the h coefficients tell us that the first term in the Hamiltonian considers the kinetic energy of the electrons in the system and their interactions with the nucleus, while the second term considers interactions between electrons.

In the final step of this procedure, we put our Hamiltonian into a form usable by VQE, by applying the *Jordan-Wigner transformation* [18]. This transformation maps products of creation and annihilation operators to products of Pauli operators. We shall not write out the general form of the Jordan-Wigner transformed Hamiltonian, as we shall see in the next section that symmetries may often be exploited which allow a Hamiltonian to be written in a much simpler form.

We are now prepared to step outside of the theory of VQE and see some of the first experimental implementations of the algorithm.

3 Experimental Implementations of VQE

The first experimental implementation of VQE was performed by Peruzzo et al., using photonic qubits [3]. The qubits in this implementation were prepared using *Spontaneous Parametric Down Conversion* (SPDC) [19], a process which creates pairs of correlated photons using a laser and a nonlinear crystal. Passing the beam of the laser through the nonlinear crystal causes the production of photon pairs, whose polarizations exhibit one of two types of correlations. In type 1 correlations, the output photons share the same polarization, while in type 2 correlations the output photons have perpendicular polarizations. In the case of the photonic VQE implementation, type 1 SPDC was used to create a $|00\rangle$ state, which was subsequently manipulated using quantum gates, to create arbitrary two-qubit pure states. With this technique, Peruzzo et al. had the means to study general 4×4 Hamiltonians.

The particular Hamiltonian investigated in [3] was that of He-H$^+$. As we previously saw, we can derive a form of this molecule's Hamiltonian which is suitable for VQE, by using the Born-Oppenheimer approximation, second quantization, and the Jordan-Wigner transformation. The Hamiltonian we receive is:

$$H(R) = \sum_{i,\alpha} h^i_\alpha(R)\sigma^i_\alpha + \sum_{i,j,\alpha,\beta} h^{ij}_{\alpha\beta}(R)\sigma^i_\alpha\sigma^j_\beta,$$

where σ^i_α refers to the Pauli operator σ_α $(\alpha = x, y, z)$, acting on particle i. As was previously alluded to, specific symmetries of the He-H$^+$ molecule were exploited to receive the above form of H.

Using the VQE algorithm, Peruzzo et al. were able to compute the ground state energy of the He-H$^+$ system for various values of R. Computing and plotting the ground state energy of this Hamiltonian for a range of R values produced the *bond dissociation curve* for the molecule - a characterization of how the molecular energy changes as the distance between the He and H$^+$ nuclei changes. The location of the minimum of this curve provides the equilibrium bond length of the molecule, found to be 92.3 ± 0.1 pm, with a corresponding electronic ground state energy of -2.865±0.008 MJ/mol. It was found that over 96% of the data points of the computed bond dissociation curve were within chemical accuracy of the theoretically predicted curve.

We next consider an implementation of VQE using trapped ion qubits [20]. In this implementation, the He-H$^+$ Hamiltonian was studied once again. However, this implementation was able to perform the necessary quantum processing using only a single trapped ion, as opposed to the two photonic qubits of the previous implementation. The ion under consideration was $^{117}Yb^+$. The procedure for writing the entire VQE algorithm onto a single trapped ion is as follows: begin by performing the same Born-Oppenheimer-second-quantization-Jordan-Wigner procedure that we are familiar with. Since He-H$^+$ was being studied once again, the same Hamiltonian as above was received. In particular, we end up with a 4×4 Hamiltonian. Such a system may be studied using two qubits - this is the procedure used in the previous implementation. However, we may also study this Hamiltonian using a single four-level system. This is the key to implementing the VQE algorithm using a single trapped ion - we construct a basis out of four energy levels of the trapped ion, labelled $|G\rangle$ (the ground state), $|E_{11}\rangle$, $|E_{12}\rangle$, and $|E_2\rangle$ [1]. Using this basis allows the He-H$^+$ Hamiltonian to be mapped onto the $^{117}Yb^+$ ion. Moreover, we may apply the Jordan-Wigner transformation to the UCCA, mapping its excitation operators into products of Pauli operators.

The form of the T operator of the UCCA for the He-H$^+$ system is $T = T_1 + T_2$, with the form of T_i, as given in Section 2.3. After applying the Jordan-Wigner transformation, the operator T is found to be 4×4, meaning that the operator $i\hbar(T - T^\dagger)$ is 4×4 as well. Recall that the UCCA may be created efficiently by evolving a Hartree-Fock ground state under the effective Hamiltonian $H_{eff} = i\hbar(T - T^\dagger)$. Since the effective Hamiltonian is also 4×4 in this case, we may map the entire creation procedure for the UCCA onto the trapped ion, as well. The form of the effective Hamiltonian, in terms of the basis energy levels of the trapped ion turns out to be

$$H_{eff} = it_3^1(|E_{11}\rangle \langle G| + |E_2\rangle \langle E_{12}|) + it_4^2(|E_{12}\rangle \langle G| + |E_2\rangle \langle E_{11}|) + it_{34}^{21} |E_2\rangle \langle G| + \text{h.c.}$$

where h.c. denotes the Hermitian conjugate and t are coefficients in the T operator of the UCCA.

Note that this form of the effective Hamiltonian is a weighted sum of energy state transitions (e.g. the first term is a transition from the ground state to the excited state $|E_{11}\rangle$). Knowing this, in order to prepare the UCCA, we need to be able to produce each of the required energy state transitions. This is in fact possible, by using a sequence of resonant microwave pulses, as outlined in [20]. The weight factors, $t_3^1, t_4^2, t_{34}^{21}$ are controlled by the durations of the pulses.

Using the VQE method, Shen et al. were able to determine the ground state energy of He-H$^+$ for a series of nuclear separations. Using their data, they were able to plot the bond dissociation curve for the molecule, obtaining an equilibrium

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[1] The subscripts in these states are not important for our purposes - they simply characterize the states of the electrons in each of the above energy levels of the $^{117}Yb^+$ ion. We use this notation only for consistency with the original paper.

bond length of 1.73 a.u. (91.5 pm), with a corresponding ground state energy of -2.86 ± 0.05 MJ/mol. Additionally, the behaviour of the ground state energy was also studied under the influence of an external electric field, by introducing additional terms into the Hamiltonian. It was found that chemical bond softening (weakening of the bond between He and H^+) occurred as the electrical field strength was increased, eventually leading to dissociation (the bond breaking between He and H^+). By comparing their results using VQE, with results using perturbation theory, it was found that the VQE algorithm produced a much more accurate prediction of the bond dissociation curve in the presence of the electric field, than second order perturbation theory. As a final application of VQE, the excited states of He-H^+ were studied, using a technique suggested in [3]: consider the new Hamiltonian $H_\lambda = (H - \lambda I)^2$, where H is the Hamiltonian of He-H^+, and λ is a tunable parameter. When λ is close to one of the energy eigenvalues of the original Hamiltonian, H, the expectation value of H_λ with respect to the corresponding excited state eigenvector, will be at a minimum. Thus the VQE algorithm can be used with this new Hamiltonian, by scanning through possible λ values. Unfortunately, this means that instead of simply searching for the state which minimizes the expectation value of a given Hamiltonian, we now must find the minimal expectation value for a series of Hamiltonians, H_λ, until we find the minimum expectation value over all λ. We will see in Section 4 that an extension of the VQE algorithm allows the computation of excited state energies in a much more straightforward manner. In the trapped ion implementation, the first three excited states of He-H^+ were investigated, but only the 3rd excited state could be resolved, due to the small energy gap between the first two excited states.

The next experimental implementation we shall examine uses superconducting qubits to perform VQE [21]. In particular, their superconducting system was based on the Xmon [22], a variation of the planar transmon qubit [23], which is in turn an extension of the Cooper Pair Box (CPB) qubit [24]. The CPB is a critical element in one type of superconducting qubit, known as the *charge qubit.* Superconducting qubits may be characterized into charge, charge-flux, flux, and phase qubits, based on the ratio E_J/E_C. In this ratio, E_J is the *Josephson coupling energy*, an energy value characteristic to a central element of superconducting qubit systems, known as a *Josephson junction*, and E_C is the electrostatic Coulomb energy of a single Cooper pair in the system. As charge qubits, CPB systems employ small E_J/E_C ratios, where E_C dominates.

CPB qubits have been a quintessential example of superconducting qubits since their invention and have been used to great effect, but despite their utility, CPB qubits are limited by their coherence times, which are insufficient for large scale quantum computation [23]. The development of the transmon was undertaken to remedy this issue. The key difference between the transmon and the CPB is that the transmon utilizes a much larger E_J/E_C ratio. The idea behind this choice, comes from the fact that both *anharmonicity* and *charge dispersion* are related to the magnitude of this ratio. Anharmonicity is a measure of how far a system is from being a harmonic oscillator. When we talk about anharmonicity in the context of quantum information, what we are particularly concerned with, is having energy levels in our system which are not of the same structure as those of the harmonic oscillator. Recall that the energy levels of the harmonic oscillator are equally spaced apart. It is difficult to force the state of such a system to remain trapped within any two particular energy levels. For qubits, two level systems are a necessity. Oftentimes we cannot construct a system which exhibits only two energy levels, and so instead, we try to force the state of the system to remain within two of its many possible energy levels. To achieve our two state system, we need to have non-constant energy level differences, so that it becomes energetically favourable for the state to remain within a two-level subsystem. A large anharmonicity (being far away from a harmonic oscillator) is thus necessary in the construction of qubits. Charge dispersion, on the other hand, is a description of the sensitivity of a system to environmental (electrical) noise. The smaller the charge dispersion, the more insensitive the qubits are to small perturbations in the system. In an optimal quantum computing system then, we would want to maximize anharmonicity while minimizing our charge dispersion. Unfortunately, it was discovered that both the anharmonicity and charge dispersion of superconducting qubits will *decrease* with an increasing E_J/E_C ratio. The beauty behind the transmon design, however, is the realization that while the charge dispersion decreases exponentially in E_J/E_C, the anharmonicity of qubits only decreases polynomially [25]. This allows us more freedom in our choice for E_J/E_C, and in particular, means that by increasing the ratio, we may be able find a value of E_J/E_C which best capitalizes on the charge dispersion, without significantly sacrificing the anharmonicity. This is the main idea behind the transmon qubit, and it has been used to great success.

The Xmon is a further extension of the CPB, building off of the transmon design, in order to focus on improving not only the coherence time of the qubit, but also to improve qubit connectivity and control. The energy coherence time of the Xmon was found to be 44 μs [22], in comparison to 9.7 μs measured for the original transmon design [26]. The emphasis on the connective properties of Xmons, refers to the fact that Xmons are designed to be easily connectable to other quantum processing components, such as quantum buses [27] or other qubits. The focus on qubit control, refers to the fact that Xmon qubits are designed to be quickly tunable, allowing for two-qubit gates to be performed quickly. In particular, it was found that high fidelity controlled-Z gates may be performed with Xmon qubits in 25 ns [28].

In the superconducting qubit implementation of VQE, two Xmon qubits were used to study the ground state energy of H_2. The form of the Hamiltonian and UCCA in this case were as follows:

$$H = g_0(R)I + g_1(R)\sigma_z^0 + g_2(R)\sigma_z^1 + g_3(R)\sigma_z^0\sigma_z^1 + g_4(R)\sigma_y^0\sigma_y^1 + g_5(R)\sigma_x^0\sigma_x^1$$

and

$$|\Psi(\theta)\rangle = \exp[-i\theta\sigma_x^0\sigma_y^1]\,|01\rangle\,.$$

where σ_α^i again refers to the αth Pauli ($\alpha = x, y, z$) acting on the ith qubit, and θ is a tunable parameter, and the g are coefficients which depend on the nuclear separation, R. Note that in this implementation, the form of the UCCA is such that there is only one tunable parameter. As such, we have renamed the one t parameter as θ, so as not to confuse it with time.

As was the case for the two previous VQE implementations, the ground state energy of the investigated molecule was studied for various bond lengths, and the bond dissociation curve was plotted. The equilibrium bond length of H_2 was found to be 0.72 Å. Moreover, the authors were able to provide the first experimental evidence that VQE is robust to systematic errors. Classical simulations were performed of the circuit employed in this implementation of VQE, in order to compute the theoretically optimal parameters for the UCCA at each bond length. It was found that when these theoretically optimal parameters were applied to the ansatz, and the ground state energy of the H_2 molecule was computed with these states, the resulting ground state energies were less accurate than the energies approximated using the experimentally determined parameters, by up to an order of magnitude. This implies that there were systematic errors present in the experimental system, which the classical simulation of the circuit was not able to capture, leading to an inaccurate value for the ground state energy when using the theoretically optimal parameters. On the other hand, the ground state energy computed using the VQE algorithm was able to circumvent these errors in a way that the theoretical computation could not, producing a more accurate ground state energy. This implies that the VQE algorithm provides a certain level of robustness to systematic errors.

4 Extensions

We have now seen three physical implementations of the VQE algorithm in its original form. In this final section of the paper, we shall consider an extension of the VQE algorithm, which utilizes ideas from QPE (quantum phase estimation) in order to best complement the benefits and limitations of VQE. In particular, this algorithm will allow us to compute both the ground and excited states of a given Hamiltonian in a very straightforward manner. This new algorithm, introduced in [29], is known as the witness assisted variational eigenspectra solver, or *WAVES protocol*. Given an appropriate Hamiltonian (i.e. one which can be written as the sum of a number of Pauli group elements which is polynomial is the size of the system), the idea of this algorithm is to compute the ground and excited states, using the entropy of the system.

We consider a two-qubit system, made up of the *control qubit*, with state ρ_C, and the *target qubit*, with state ρ_T. We then define the *objective function*:

$$F_{obj} = E + TS(\rho_C)$$

where E is the energy estimate found by taking the expectation value of the Hamiltonian with respect to the target qubit (reminiscent of standard VQE), T is a tunable parameter, and $S(\rho_C)$ is the Von Neumann entropy of the control qubit. This definition for the objective function was chosen to be analogous to the *Helmholtz free energy* of thermodynamics, defined as $U - TS$, where U, T, and S are the internal energy, temperature, and entropy of the system, respectively.

Note that the control qubit's state may be found using quantum state tomography [30]. Once the tomography is performed, the Von Neumann entropy of the state may be determined. As the energy estimate E may be computed using the standard VQE techniques laid out in Section 2, the objective function may be computed in a relatively straightforward manner.

The key insight to the WAVES protocol is that the entropy of the control qubit will go to zero whenever the target qubit is in *any* eigenstate of the Hamiltonian. This is what allows the protocol to be able to estimate the ground and excited state energies. Consider the case of the ground state energy. At any value of T, the absolute minimum of the objective function is obtained at the ground state, since at this point, E obtains its minimum value, and $S(\rho_c) = 0$. However, we need to be a bit more careful when considering excited states. The value of the objective function obtained at an excited state, $F_{obj} = E_{excited} + 0$ may actually turn out to be larger than the value of the function for some non-eigenstate, $F_{obj} = E' + TS(\rho_C)$, when T is sufficiently small. It is thus crucial in this case to choose a value for T that is large enough so that the objective function will obtain local minima for excited eigenstates. We thus consider the high-T limit when searching for excited states of our system. Due to its role in uncovering the energy eigenstates of the system, the entropy of the control qubit is known as an *eigenstate witness*.

In order to perform our variational procedure on the objective function, we need to begin with some ansatz state which depends on a set of parameters, just as in VQE. For convenience, we may consider the UCCA once more. We then perform a variational search to obtain the minimum value of F_{obj}, and thus the ground state energy of the system. Next we move to the high-T limit and perform another variational search for each excited state that we wish to find. Our initial state for each of these variational searches is taken to be the ground state found with the preliminary search, with a system-dependent perturbation applied. These perturbations take the form of unitary matrices U_i, one for each energy eigenstate. Concretely, the perturbations are of the form $U = \exp[\pi/2(\hat{a}_i^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{a}_i)]$, for some i, j. We can perform the Jordan-Wigner transformation on these states, to obtain these perturbations in terms of Pauli matrices, which can then be easily implemented using quantum circuits. The idea behind performing these perturbations is as follows: many-body Hamiltonians, such as those describing atoms or molecules, are of the form $H = H_0 + V$, where $H_0 = \sum_i h_{ij} \hat{a}_i^\dagger \hat{a}_j$ describes the energies of single particles, and V describes the interaction energies of the system. We saw this form of Hamiltonian when we considered the Born-Oppenheimer approximated electronic Hamiltonian in Section 2.4. It is known that H_0 is the dominant term in this expansion, and thus the behaviour of energy eigenstates can be approximated as only coming from single particle excitation terms. In particular, transitions from the ground state to an excited-state are approximated as perturbations which depend only on single excitation operators, $\hat{a}_i^\dagger \hat{a}_j$. In order to obtain unitary perturbations, these single excitation operators are written as an anti-Hermitian combination, and exponentiated, and thus we arrive at $U = \exp[\pi/2(\hat{a}_i^\dagger \hat{a}_j - \hat{a}_j^\dagger \hat{a}_i)]$.

Once we have completed our search for excited states, we can move on to the final step in the procedure: refining our estimations for the ground and excited state energies. This is done by performing *iterative phase estimation* (IPE) [31], where we use the energy eigenstates obtained in the first and second steps of the WAVES protocol as input into the IPE algorithm. We previously discussed the ideas behind QPE. IPE is a similar procedure, which achieves the same result - estimating the eigenvalues of a unitary matrix - but in a slightly different manner. The QPE algorithm runs for a certain number of iterations, and at the end of those iterations outputs an estimate for an eigenvalue of the input matrix. IPE estimates the eigenvalue one digit at a time - from least significant to most significant digit.

Santagati et al. experimentally demonstrated the WAVES procedure by studying the energy spectrum of a two-chlorophyll system. The computation was performed using a two-qubit silicon quantum photonic chip as its quantum processor. The chip used spontaneous four wave mixing to produce its qubits. This is a process which converts two pump photons (photons provided by a laser, as input) to an entangled pair of photons, called the *signal* and *idler* photons. As energy is conserved in this process, the energies of the signal and idler photons add to total energy of the two incident pump photons, and by convention, the output photon with the larger frequency is denoted the signal photon. Through a filtering process based on photon energies, the signal photon was found and selected to be the control qubit in the WAVES procedure, while the idler qubit was chosen to be the target qubit. The ground state and a single excited state were studied in this implementation. The perturbation applied in this implementation of the WAVES procedure was of the form $U = e^{i\pi\sigma_z/2}$. It was found that when the experimentally obtained ground and excited state wave functions were compared to the theoretically predicted ones, the fidelity (defined as $|\langle\psi_{exp}|\psi_{theor}\rangle|^2$) was $99.48 \pm 0.28\%$ and $99.95 \pm 0.05\%$, for the ground and excited state wave functions, respectively. Additionally, numerical simulations were performed to study how the WAVES protocol would fare when considering more complex systems. In particular, Santagi et al. were concerned with the response of the protocol to the appearance of local minima in the objective function. Using the systems, H_2, H_3^+, H_3, and H_4, this concern was examined. It was found that the WAVES protocol was able to consistently find both the ground and excited states in all of the examined systems.

In the ion trap implementation of Section 3, we examined how excited states may be approximated in standard VQE, by studying the extended Hamiltonians $H_\lambda = (H - \lambda I)^2$. We found that this approach comes with an extra computational cost: in order to compute the excited state energies using H_λ, we have to minimize the expectation value of H_λ for a range of λ, until we converge on a local minimum, which would correspond to an excited state energy. In contrast, WAVES is able to estimate excited state energies without introducing any extra complexity in comparison to estimating the ground state. This alone makes the WAVES protocol an enticing tool. Another advantage of this protocol in comparison to similar methods, comes from the introduction of entropy measurements as means of finding energies. The fact that entropy is an eigenstate witness in the WAVES protocol gives this procedure twice as many methods as VQE to test the algorithm's success: in both VQE and WAVES, the expectation value energy estimate, E, is minimized in order to determine the ground state energy of the system. However in WAVES, we also have that the entropy of the control qubit should go to zero when the target qubit is in the ground state. This extra check allows the WAVES protocol to be more aware of false convergences in the form of local minima of E, than standard VQE. The cost of the WAVES protocol comes in two forms: the first is the appearance of an extra (control) qubit, which must be properly stored and manipulated. The second cost of the protocol is its reliance on perturbing unitaries, U_i, when finding the excited states of the system. Though system properties were outlined in [29] which may be used to deduce the appearance of these perturbations [32], it is not clear that these properties will always provide sufficiently accurate perturbations, and other methods for determining these perturbations may be necessary in complex systems.

5 Conclusion

In this paper we have explored the variational quantum eigensolver protocol, both in terms of its theory and experimental implementations. The theoretical framework of the protocol was developed by studying its inspirations in variational calculus, as well as computational and quantum chemistry. Physical implementations of the VQE algorithm, using photonic, ion trap, and superconducting qubits, were discussed in terms of their design and results. Finally, an extension of the original VQE algorithm was studied, which can be used to compute both the ground and excited states of a molecular Hamiltonian in a straightforward manner.

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