Some Open Questions Concerning Hybrid Quantum Eigensolvers

1 Background:

It is widely agreed that the accurate simulation of quantum many-body physics is one of the most exciting applications of sophisticated quantum algorithms such as quantum phase estimation (QPE) [3]. Unfortunately, despite promising experimental advances in recent years, present quantum devices continue to suffer from the issue of decoherence, which prevents the practical execution of such algorithms.

Hybrid quantum algorithms such as the variational quantum eigensolver (VQE) [4] in which a quantum subroutine is incorporated within a largely classical numerical method were originally developed as an alternative that would, perhaps, be better suited for implementation on near-term quantum devices. Despite initial excitement, recent research indicates that the VQE suffers from at least two major issues that prevent its execution on near-term quantum devices for quantum systems of chemical and physical interest. These issues are (i) the huge number of *measurements* that must be performed on the quantum device to obtain statistical averages of the variational energy [8] and (ii) the difficulty of the associated optimisation problem which involves a cost function that may become exponentially flat with increasing system size [1].

As a consequence of this situation, two broad research directions have developed. The first advocates for a return to quantum algorithms such as QPE and focuses on the optimisation of the individual steps within such algorithms to reduce the quantum resources required for their execution while waiting for the development of fault-tolerant, error-corrected quantum hardware. The second direction focuses instead on the continued development of alternative hybrid quantum algorithms suited to near-term quantum devices with the hope that some form of quantum advantage can still be leveraged from these algorithms in the short term. Note that advocates of this later approach have an additional justification: a necessary pre-requisite for algorithms such as QPE is the availability - on the quantum computer - of a trial state that is a reasonable approximation of the sought-after ground state of the quantum system under study [3]. Therefore, even after the advent of error-corrected quantum computers, hybrid algorithms could find use as state-preparation algorithms required to successfully run a QPE routine.

In the present project, we choose to take the second route mentioned above by attempting to answer some basic mathematical questions regarding the so-called projective quantum eigensolver proposed by Stair and Evangelista [6]. Let us now briefly present this algorithm.

2 Problem Setting:

Given a quantum system with Hamiltonian H that acts on a Hilbert space $\mathcal{H}$ with inner product $\langle \cdot, \cdot \rangle$ and associated norm $\| \cdot \|$, we seek to find the lowest eigenvalue

$$E_0 := \min_{0 \neq \Phi \in \mathcal{H}} \frac{\langle \Phi, H\Phi \rangle}{\|\Phi\|^2}. \tag{1}$$

Let now $\{\Psi_0\} \cup \{\Psi_\mu\}_{\mu \in \mathcal{I}}$ be an orthonormal basis for $\mathcal{H}$ with Ψ_0 denoting a state that is easy to prepare on quantum hardware. If we assume that the sought-after lowest eigenvalue is *simple* with associated (normalised) eigenvector $\Phi_0 \in \mathcal{H}$, then it follows that there exists a unitary operator $\mathcal{U} \colon \mathcal{H} \to \mathcal{H}$ with the property that

$$\mathcal{U}\Psi_0 = \Phi_0 \qquad \text{so that} \qquad H\mathcal{U}\Psi_0 = H\Phi_0 = E_0\Phi_0 = E_0\mathcal{U}\Psi_0 \tag{2}$$

This in turn implies that

$$\mathcal{U}^\dagger H \mathcal{U}\Psi_0 = E_0 \mathcal{U}^\dagger \mathcal{U}\Psi_0 = E_0\Psi_0,$$

leading to the set of projected equations

$$\begin{cases} \langle \Psi_\mu,\, \mathcal{U}^\dagger H \mathcal{U}\Psi_0 \rangle & = 0 \\ \langle \Psi_0,\, \mathcal{U}^\dagger H \mathcal{U}\Psi_0 \rangle & = E_0^* \end{cases} \tag{3}$$

Assuming that the Hilbert space $\mathcal{H}$ is of dimension $M+1$, Equation (3) represents a system of M equations that must be satisfied by the unitary operator $\mathcal{U}$ together with an additional equation to determine the ground state eigenvalue E_0^*. Of course, thus far, no numerical method has really been presented since there are many such unitary operators $\mathcal{U}$ which satisfy the relations (2)-(3), and - in any case - finding such a $\mathcal{U}$ is as difficult as solving the minimisation problem (1).

The main idea of the projective quantum eigensolver is now to introduce a *parameterised* unitary operator $\mathcal{U}(\mathbf{t})$ with parameter $\mathbf{t} \in \mathbb{R}^d$, $d \ll M$ together with a suitable subset of d basis elements $\{\Psi_\nu\}_{\nu \in \mathcal{K}} \subset \{\Psi_\mu\}_{\mu \in \mathcal{I}}$, $|\mathcal{K}| = d$. We then seek $\mathbf{t}_0 \in \mathbb{R}^d$ that satisfies

$$\mathbf{r}_\nu(\mathbf{t}_0) := \langle \Psi_\nu,\, \mathcal{U}^\dagger(\mathbf{t}_0) H \mathcal{U}(\mathbf{t}_0)\Psi_0 \rangle = 0 \qquad \forall \nu \in \mathcal{K}. \tag{4}$$

Equation (4) is now a system of d equations for d unknowns and, hopefully, possesses a solution that is computationally tractable to approximate. Once this solution $\mathbf{t}_0$ has been computed, the associated variational energy is given by

$$E_0^{\text{approx}} = \langle \Psi_0,\, \mathcal{U}^\dagger(\mathbf{t}_0) H \mathcal{U}(\mathbf{t}_0)\Psi_0 \rangle.$$

Some practical questions now remain, namely, how to choose the parameterised unitary operator $\mathcal{U}(\mathbf{t})$, how to select the set of states $\{\Psi_\nu\}_{\nu \in \mathcal{K}}$, and how to implement the method on quantum hardware. A typical choice for the unitary operator $\mathcal{U}(\mathbf{t})$ is the so-called disentangled unitary coupled cluster (d-UCC) ansatz, in which $\mathcal{U}(\mathbf{t})$ for $\mathbf{t} = \{t_\nu\}_{\nu \in \mathcal{K}} \in \mathbb{R}^d$ takes the form

$$\mathcal{U}(\mathbf{t}) = \prod_{\nu \in \mathcal{K}} \exp\Big(t_\nu \big(\widehat{\tau}_\nu - \widehat{\tau}_\nu^\dagger \big) \Big). \tag{5}$$

Here, each $\widehat{\tau}_\nu$ is a so-called particle-hole excitation operator that maps the reference state Ψ_0 to the state Ψ_ν, $\widehat{\tau}_\nu^\dagger$ denotes its adjoint, and we refer to the sum $\widehat{\tau}_\nu - \widehat{\tau}_\nu^\dagger$ as an evolution operator. We also

emphasise that the product is over all indices $\nu \in \mathcal{K}$. Let us also highlight that the exact choice of indices, i.e., exactly which excitation operators to include in the ansatz as well as their order can be made in an adaptive manner. Such an adaptive strategy has been proposed in [6]. Additionally, as shown in this reference, with this choice of ansatz for the unitary operator $\mathcal{U}(\mathbf{t})$, it is possible to estimate all equation residuals $\{\mathbf{r}_\nu(\mathbf{t})\}_{\nu\in\mathcal{K}},\ \mathbf{t} \in \mathbb{R}^d$ using $2d+1$ measurements of the expectation value of the Hamiltonian H for relatively simple trial quantum states. Equipped with these ingredients, one can now approximate solutions to the non-linear equation (4) using, e.g., a quasi-Newton method. We refer to [5] for an excellent description of such approaches supplemented by an error analysis.

3 Aims of the project:

The goal of this project is to build on the work undertaken in [5, 6] and further the analysis of the projective quantum eigensolver. In particular, we are interested in answering the following questions:

- What are the approximability properties of the d-UCC ansatz? More precisely, given some $d \in \mathbb{N}$ and the exact ground state Φ_0, can we estimate the quantity

$$\underset{\substack{\mathbf{t}\in\mathbb{R}^d \\ (\nu_1,\ldots,\nu_d)\in\mathcal{I} \\ \nu_i\neq\nu_j\forall i,j}}{min} \left\| \Phi_0 - \prod_{\nu\in\mathcal{K}} \exp\left(t_\nu\left(\widehat{\tau}_\nu - \widehat{\tau}_\nu^\dagger\right)\right)\Psi_0 \right\|.$$

  Moreover, if $d \in \mathbb{N}$ is fixed, how does this quantity change as the dimension of the underlying Hilbert space $\mathcal{H}$ grows, or if we allow repetitions of excitation operators in the ansatz? The best existing result we are familiar with is given in [2] but this result states only that an arbitrary wave-function in the Hilbert space $\mathcal{H}$ of dimension $M+1$ can be written as a disentangled product of Mevolution operators. For obvious reasons, this result is not very practical since it suggests the number of terms in the disentangled product (5) should linearly in M, and therefore exponentially with the number of qubits n (since, typically, $M = 2^n$).

- For a given choice of d-UCC ansatz, under what conditions can we prove well-posedness of the resulting non-linear system of equations (4)?

- Is it possible to develop a better adaptive strategy for the choice of indices $\nu \in \mathcal{K}$ with which to form the unitary operator $\mathcal{U}(\mathbf{t})$? Moreover, can we develop an error and measurement balancing strategy in the following sense: at each iteration of the algorithm, can we have mathematically-justified criteria that inform us whether it is better to perform a quasi-Newton iteration to reduce the residues $\mathbf{r}_\nu$ for $\nu \in \mathcal{K}$, or it is better to enlarge the index set $\mathcal{K}$. To answer this question, we can make use of the error estimates already developed in [5] as well as previous error balancing strategies proposed for simpler problems (see, e.g., [7]).

- Are the quasi-Newton schemes proposed in [5, 6], the best algorithms for solving Equation (4)? In particular, can we use better approximations of the Jacobian as a preconditioner in order to accelerate the convergence of the scheme? This question is particularly relevant for strongly correlated systems for which a diagonal preconditioner might be a sub-optimal choice.

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