Symmetry breaking slows convergence of the ADAPT Variational Quantum Eigensolver

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Abstract—The accurate treatment of molecular systems exhibiting strong electronic correlations has long been a target of quantum simulation. Strong correlation often results in symmetry-breaking of the mean-field reference, leading to Löwdin’s “symmetry dilemma”[1] whereby accuracy in the energy can be increased by breaking intrinsic symmetries of the system. We explore the impact of symmetry breaking on the performance of ADAPT-VQE using two strongly correlated systems where increasing correlation leads to spontaneous symmetry breaking of the mean-field solutions. We analyze the role that symmetry breaking in the reference states and orbital mappings of the fermionic Hamiltonians have on the performance of ADAPT-VQE. We observe that breaking symmetry has a deleterious effect on ADAPT-VQE by increasing the length of the ansatz necessary for energy convergence and exacerbating the problem of “gradient troughs”.

I. INTRODUCTION

Simulating chemical systems on quantum hardware offers a potentially attractive alternative to classical simulations, as the combinatorial growth of the Hilbert space is absorbed by the quantum processor[2, 3]. In the noisy intermediate scale quantum (NISQ) era, however, the size and reliability of modern quantum devices require careful design of algorithms to cope with their shortcomings[4].

The Variational Quantum Eigensolver (VQE) offers an approach for quantum simulation of chemical Hamiltonians[5]. In this scheme, one prepares parameterized trial states $|\psi(\vec{\theta})\rangle$ on the quantum processor and minimizes the expectation value of the Hamiltonian with respect to the ansatz parameters. The accuracy of a VQE is ultimately limited by the variational flexibility of the predefined ansatz.

The adaptive problem-tailored VQE (ADAPT-VQE) method avoids a predefined unitary ansatz by constructing an arbitrarily accurate quasi-optimal ansatz on the fly as informed by the Hamiltonian[6]. ADAPT-VQE has been shown to both provide smaller gate counts and errors than traditional VQE methods[6, 7].

A motivation for the adaptive construction of ansätze is the ability to treat systems that are strongly correlated, where the performance of traditional VQEs is expected to suffer. In this work, we apply ADAPT-VQE to two systems that display variable amounts of strong correlation: (i) the fermionized anisotropic Heisenberg model, where the anisotropy parameter allows for control over the level of correlation in the system, and (ii) the symmetric dissociation of linear $H_2$. In both of these cases, increasing the level of correlation of the system leads to spontaneous symmetry breaking (parity and $S^2$, respectively) of the mean-field solutions. We explore the roles played by these symmetries, both in the reference state and the operator pool, for ADAPT-VQE, highlighting their importance in generating compact ansätze and preventing premature convergence of the algorithm.

II. METHODOLOGY

A. ADAPT-VQE Algorithm

ADAPT-VQE iteratively grows a problem-tailored unitary ansatz from a reference state by adding operators from an operator pool $\{\hat{A}_k\}$. To grow the ansatz, the current trial state, $|\psi^{(n)}\rangle$, is prepared on the device and the gradient of the energy with respect to the operator parameters $\theta_k$ for each operator $\hat{A}_k$ in the pool is computed by measuring the expectation value of commutator of the Hamiltonian and the operators for the current state:

$$\frac{\partial E^{(n)}}{\partial \theta_k} = \langle \psi^{(n)} | [\hat{H}, \hat{A}_k] | \psi^{(n)} \rangle.$$ (1)

The operator corresponding to the largest gradient magnitude is then used to form the new trial state ansatz:

$$|\psi^{(n+1)}\rangle = e^{\theta_{n+1}\hat{A}_{n+1}}|\psi^{(n)}\rangle$$ (2)

The new ansatz is then optimized over all $\hat{A}_{n+1}$ via a VQE subroutine to yield $|\psi^{(n+1)}\rangle$. From here the algorithm repeats by returning to the operator gradient measurement step. Convergence of the ADAPT-VQE algorithm is typically determined by the norm of the operator gradient.

B. Fermionized Anisotropic Heisenberg Model

Spin Hamiltonians can be used in the context of chemistry to develop a coarse-grained understanding of certain molecular interactions, such as the interactions between open-shell metal atoms in multi-metal organometallic complexes.

The anisotropic Heisenberg model has a Hamiltonian given by

$$\hat{H}\text{aniso} = -2J \sum_{\langle ij \rangle} \left( \hat{S}^x_i \hat{S}^x_j + \hat{S}^y_i \hat{S}^y_j \right) - 2K \sum_{\langle ij \rangle} \hat{S}^z_i \hat{S}^z_j.$$ (3)

The anisotropic Heisenberg Hamiltonian is “fermionized” via Jordan-Wigner transformation. Beginning at the isotropic point and for all larger $K/J$, Hartree-Fock (HF) is seen to break spatial (parity) symmetry. In the first set of results, we apply ADAPT-VQE to the fermionized anisotropic Heisenberg model to investigate the role of parity symmetry in the performance of ADAPT-VQE.

We survey correlation parameter values $K/J$ ranging from 0.001 to 100. At each value of $K/J$ surveyed, we perform five ADAPT-VQE simulations using different orbital representations [Hartree-Fock (HF), broken-symmetry HF (BS-HF), local, symmetry-adapted linear combinations (SALC)] and reference states (HF, BS-HF, Néel, cat^+). Here the HF and SALC orbitals are symmetry preserving while the BS-HF and local orbitals are symmetry breaking. Similarly, the HF and cat^+ reference states are symmetry preserving while the BS-HF and Néel reference states are symmetry breaking.

C. Linear $H_4$

For linear $H_4$, we survey H–H separations from 0.50 Å to 3.00 Å. At each geometry surveyed, we compare the performance of ADAPT-VQE when performed with spin-restricted HF (rHF) and spin-unrestricted HF (uHF) orbitals. For rHF we further explore the impact of spin-adapting the operator pool, by using both the singlet-GSD

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A. Fermionized Anisotropic Heisenberg Model

As seen in Fig. 1, the use of symmetry preserving orbital bases and reference states (HF, SALC/cat+) reduces the number of ADAPT-VQE iterations required to tightly converge the energy. This reduced number of operator additions arises from the need to parameterize a smaller subspace states, whereas the symmetry breaking methods must span the full space to converge to the exact result. Therefore despite the BS-HF reference energy being much lower than the HF reference energy, the slower convergence of the former is quickly outpaced.

From the lower panel of Fig. 1, we also observe that symmetry breaking worsens a phenomena in ADAPT-VQE known as “gradient troughs”. For both broken symmetry reference states (BS-HF and Néel), the gradient norm is seen to decrease gradually as operator are added to the ansatz and then suddenly jump, corresponding to the end of an energy plateau. In these cases, the gradient trough is arising due to a lack of variational flexibility in the ansatz to restore symmetry. This issue of gradient troughs is more pernicious as excited states become quasi-degenerate with the ground state. The presence of a contaminant state in the ADAPT-VQE trial state leads to this suppression of the gradient due to an energy difference term in the expanded gradient:

$$\psi^{(n)} = \sum_{i} c_i^{(n)} \psi^{FCI}_i,$$

$$\frac{\partial E}{\partial \theta_k} = \sum_{ij} c_i^{(n)} c_j^{(n)} (E_i - E_j) \langle \psi^{FCI} | \hat{A}_k | \psi^{FCI} \rangle.$$  

By using symmetry preserving orbitals and reference states, however, this contamination is limited to only states with the same symmetry as the ground state, mitigating the problem of gradient troughs.

B. Linear $H_4$

For $H_4$, spin symmetry breaking slows the energy convergence of the ADAPT-VQE algorithm, with the rHF reference and sGSD operator pool requiring less than half of the number of operators to converge as the uHF case. Furthermore, when starting from a rHF reference state, ADAPT-VQE with a symmetry-agnostic operator pool is observed to spontaneously break the spin symmetry of the reference, leading to slower convergence of the energy as compared to the symmetry-adapted pool.

As H–H separation increases, all three ADAPT-VQE variants exhibit gradient troughs due to the presence of low-lying excited states. However, as is the case with the fermionized anisotropic Heisenberg model, ADAPT-VQE using a symmetry preserving reference state and operator pool has the shallowest gradient trough. This is due to a limitation of the number of intruder states present in the ADAPT-VQE trial state. For the rHF/uGSD case, however, the use of the symmetry breaking operator pool introduces contamination from states of different symmetries, giving rise to a deep gradient trough.

IV. CONCLUSION

Despite an energetic benefit from breaking symmetry at the level of the reference state, the use of broken symmetry reference states and/or operator pools slows the convergence of ADAPT-VQE as the system becomes more strongly correlated. Furthermore, broken symmetries are seen to exacerbate the problems of gradient troughs in ADAPT-VQE. These gradient troughs can lead to premature convergence of the algorithm when using a gradient-based convergence criteria. The use of symmetry preserving reference states is also shown to reduce the presence of contaminant states in the ADAPT-VQE trial state, while symmetry preserving pools prevent ADAPT-VQE from introducing these states into the ansatz.

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