Using VQE to Find Ground State Energy of LiH Molecule with Parity Mapping and Exploiting the Symmetry of Molecule to Reduce the Number of Qubits Required for Simulation

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Abstract

We test the parity mapping algorithm of VQE to solve the ground state energy of the LiH molecule. We further use the two qubit reduction by sing the Z_2 logical symmetry to reduce the no. of qubits and compare with the exact energy. Further, we exploit the more general point group symmetries of the molecule to taper off more qubits for the simulation using QML package of pennylane. We present our results followed by the conclusion

Contents

1   Introduction

In its most general description, VQE aims to compute an upper bound for the ground-state energy of a Hamiltonian, which is generally the first step in computing the energetic properties of molecules and materials. The study of electronic structures is a critical application for quantum chemistry and condensed matter physics. The scope of VQE is very wide-ranging and potentially relevant for drug discovery, material science, and chemical engineering. The VQE starts with an initialized qubit register. A quantum circuit is then applied to this register to model the physics and entanglement of the electronic wave function. A Quantum circuit refers to a pre-defined series of quantum operations that will be applied to the qubits. The number of consequential operations in a circuit is referred to as depth. This circuit is defined by two parts: a structure, given by a set of ordered quantum gates, often referred to as an 'ansatz', and a set of parameters that dictates the behavior of some of these quantum gates. Once the quantum circuit has been applied to the register, the state of the qubits is designed to model a trial wave function. The Hamiltonian of the system studied can be measured with respect to this wave function to estimate the energy. The VQE then works by variationally optimizing the parameters of the ansatz to minimize this trial energy, always constrained to be higher than the exact ground state energy of the Hamiltonian by virtue of the variational principle.

Provided a Hamiltonian $\hat{H}$, and a trial wavefunction $|\psi\rangle$, the ground state energy associated with this Hamiltonian, E0,is bounded by

$$E_0 \leq \frac{\langle\psi|\,\hat{H}\,|\psi\rangle}{\langle\psi|\psi\rangle}$$

The objective of the VQE is, therefore to find a parameterization of $|\psi\rangle$, such that the expectation value of the Hamiltonian is minimized. This expectation value forms an upper bound for the ground state energy and, in an ideal case, should be indistinguishable from it to the level of precision desired.We hence express $|\psi\rangle$ as the application of a generic parametrized unitary $U(\theta)$ to an initial state for N qubits, with θ denoting a set of parameters taking values in $(\pi, \pi]$. we can now write the VQE optimization problem as

$$E_{VQE} = \min_{\theta} \langle 0|\, U^{\dagger}(\theta)\hat{H}U(\theta)\,|0\rangle$$

This eq. is also referred to as the cost function of the VQE optimization problem, which is a terminology inherited from the machine learning and optimization literature. We can continue this description by writing the Hamiltonian in a form that is directly measurable on a quantum computer, as a weighted sum of spin operators . Observables suitable for direct measurement on a quantum device are tensor products of spin operators (Pauli operators). We can define these as Pauli strings: $\hat{P}_a \in \{I, X, Y, Z\}^{\otimes N}$, with N the number of qubits used to model the wavefunction. The Hamiltonian can be: rewritten as

$$\hat{H} = \sum_a^{\mathcal{P}} w_a \hat{P}_a$$

with w_a a set of weights, and $\mathcal{P}$ the number of Pauli strings in the Hamiltonian. The minimization becomes

$$E_{\text{VQE}} = \min_{\theta} \sum_a^{\mathcal{P}} w_a \left\langle \mathbf{0} \left| U^{\dagger}(\boldsymbol{\theta})\hat{P}_a U(\boldsymbol{\theta}) \right| \mathbf{0} \right\rangle,$$

where the hybrid nature of the VQE becomes clearly apparent: each term $E_{P_a} = \left\langle \mathbf{0} \left| U^\dagger(\boldsymbol{\theta}) \hat{P}_a U(\boldsymbol{\theta}) \right| \mathbf{0} \right\rangle$ corresponds to the expectation value of a Pauli string $\hat{P}_a$ and can be computed on a quantum device, while the summation and minimization $E_{VQE} = \min_\theta \sum_a w_a E_{P_a}$ is computed on a conventional computer.

In brief, the pipeline for VQE can be written as, as discussed in [5]:

- Hamiltonian construction and representation

- Encoding of operators

- Measurement strategy and grouping

- Ansatz and state preparation

- Parameter optimization

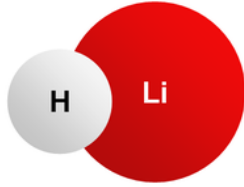## 2 The Symmetry of LiH Molecule

Figure 1: Lithium Hydride Molecule

Each molecule has a symmetry operation that define the molecule's overall symmetry. These sets of symmetry are known as a point group. There are various type of point groups like as (Group C1,Ci,Cs),(Group Cn,Cnh,Cnv,C∞v),(Group Dn,Dnd,Dnh,D∞v),Sn Groups, Cubic Group(Tetrahydral, Octahedral,Icosahedral).

Molecules Containing C1 Group has only identity and those molecules have no symmetry, they are asymmetric molecules. Molecules containing Ci group have identity and a center of inversion i and Molecules containing Cs group have identity and a plane of reflection σ. So, Group(C1,Ci,Cs) is Non rotational Group which represent the lowest symmetry Group.

Molecules containing Cn Group have n fold principal axis rotaion and identity.Molecules containing Cnh Group have n fold principal axis rotation and a horizontal plane σ_h . Molecules contining Cnv Group have n fold principal axis Rotation and one vertical plane of reflection σ_v. Molecules containing C∞v group have two infinity fold principal axis and infinity verical mirror plane. So, Group(Cn,Cnh,Cnv,C∞v) is rotational group symmetry.

LiH is linear Molecule. So, it belongs to C∞v point group. So, Lithium Hydraide contains two ∞ fold procipal axis rotation and infinity vertical mirror plane σ_v and it has symmetry element E. This point group symmetry can be used to taper off qubits similarly like tapring qubits using Z_2 symmetries, as prescribed in [4].

3 Reducing The Number of Qubits using Symmetry: Qubit Tapering

The performance of variational quantum algorithms is considerably limited by the number of qubits required to represent wave functions. In the context of quantum chemistry, this limitation hinders the treatment of large molecules with algorithms such as the variational quantum eigensolver (VQE). Several approaches have been developed to reduce the qubit requirements for quantum chemistry calculations. In this tutorial, we demonstrate the symmetry-based qubit tapering approach which allows reducing the number of qubits required to perform molecular quantum simulations based on the Z_2 symmetries present in molecular Hamiltonians.

A molecular Hamiltonian in the qubit basis can be expressed as a linear combination of Pauli words as

$$H = \sum_{i=1}^{r} h_i P_i$$

where h_i is a real coefficient and P_i is a tensor product of Pauli and identity operators acting on M qubits

$$P_i \in \pm \{I, X, Y, Z\}^{\otimes M}$$

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The main idea in the symmetry-based qubit tapering approach is to find a unitary operator U that transforms H to a new Hamiltonian H which has the same eigenvalues as H.

$$H = U^\dagger H U = \sum_{i=1}^{r} c_i \mu_i,$$

such that each μ_i term in the new Hamiltonian always acts trivially, e.g., with an identity or a Pauli operator, on a set of qubits. This allows tapering-off those qubits from the Hamiltonian.

More generally, we can construct the unitary U such that each μ_i term acts with a Pauli-X operator on a set of qubits $\{j\}$, $j \in l, \therefore, k$ where j is the qubit label. This guarantees that each term of the transformed Hamiltonian commutes with each of the Pauli-X operators applied to the j-th qubit:

$$[H, X^j] = 0,$$

and the eigenvectors of the transformed Hamiltonian H are also eigenvectors of each of the X_j operators. Then we can factor out all of the X_j operators from the transformed Hamiltonian and replace them with their eigenvalues ± 1. This gives us a set of tapered Hamiltonians depending on which eigenvalue ± 1 we chose for each of the X_j operators. For instance, in the case of two tapered qubits, we have four eigenvalue sectors: [+1,+1] , [-1,+1] , [+1,- 1] , [-1,-1].

In these tapered Hamiltonians, the set of j, $j \in l, ..., k$ qubits are eliminated. For tapered molecular Hamiltonians, it is possible to determine the optimal sector of the eigenvalues that corresponds to the ground state. This is explained in more detail in the following sections. The unitary operator U can be constructed as a Clifford operator.

$$U = \prod_{j} \left[\frac{1}{\sqrt{2}} (X^{q(j)} + \tau_j) \right],$$

where τ denotes the generators of the symmetry group of H and X^q operators act on those qubits that will be ultimately tapered off from the Hamiltonian. The symmetry group of the Hamiltonian

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is defined as an Abelian group of Pauli words that commute with each term in the Hamiltonian (excluding -I). The generators of the symmetry group are those elements of the group that can be combined, along with their inverses, to create any other member of the group. We can taper those operators that is those qubits in the measurements with their eigenvalues.

4 The Results

As mentioned in the title, the goal of this work to present the ground state simulation of the 'LiH' molecule. The ground state can be obtained using the VQE simulator of 'Qiskit'.

4.1 Using Parity Mapping

We first calculate the ground state energy using 'Parity Mapping' only. We do it for a number of separation between Li and H atom and therefore, see the variation of the simulated ground state energy with the inter atomic distance. The minimum energy corresponding to this configurations is the ground state energy, and the distance is the equilibrium distance. We see that the minimum
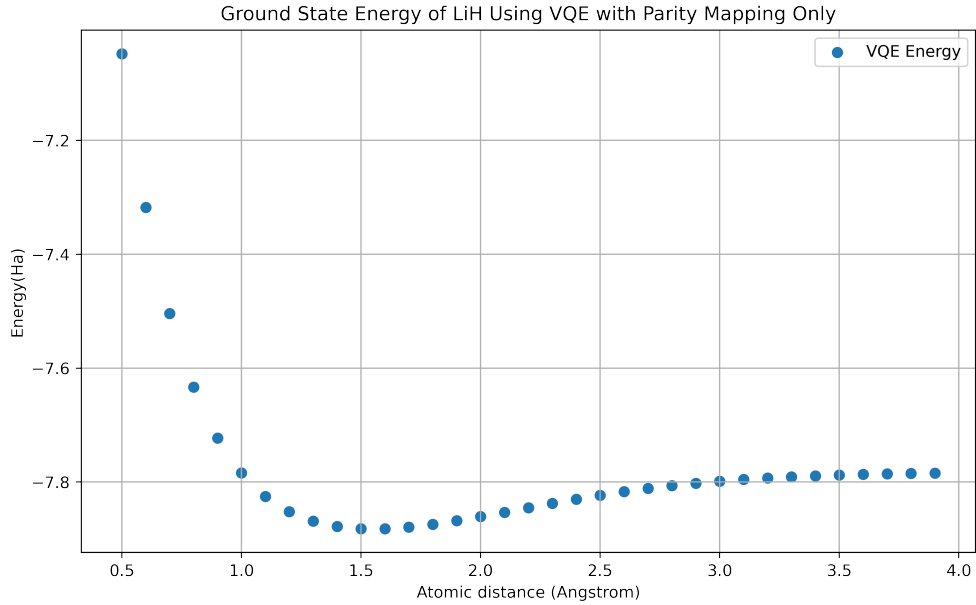

Figure 2: The Ground State Energy Simulation using Parity Mapping Only

energy is when the interatomic distance is 1.5 Angstrom and the corresponding energy is -7.88214 Ha. The python notebook used for simulation can be found at this link.

4.2 The Two Qubit Reduction

The Two Qubit Reduction is just the enhanced version of the Parity Mapping, where the Z_2symmetry logic in Qiskit is used to find additional symmetries of the Hamiltonian and thereby, by parity mapping we already have at least 2 qubits tapered off since, we already know the operators and can replace them with their eigenvalues. We use the two qubit reduction with parity mapping to find the ground state similarly. WE see that, using the two qubit reduction gives the same results, but
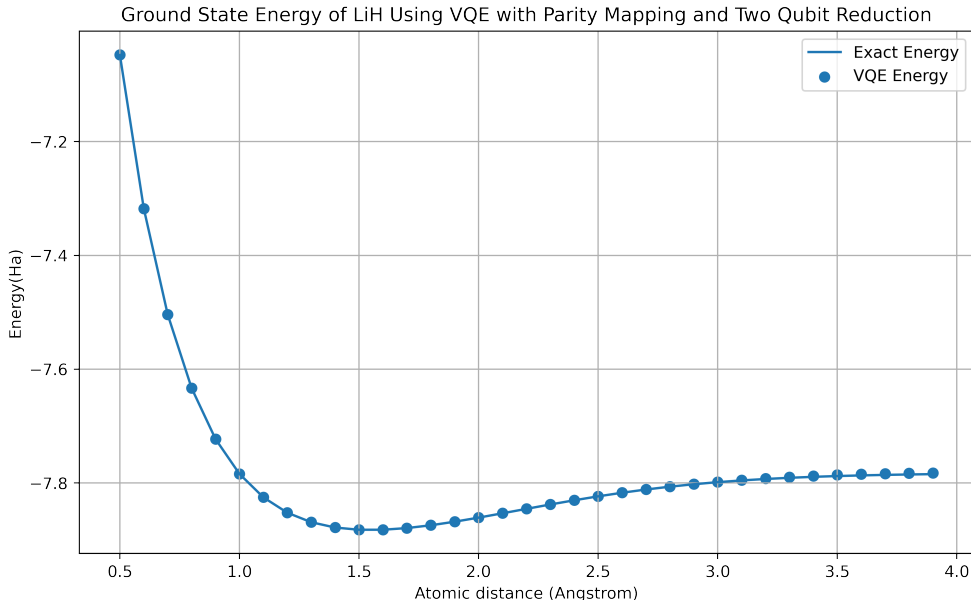

Figure 3: The Ground State Energy Simulation using Parity Mapping Two Qubit Reduction

now two qubits have been tapered off from the Pauli String. The results are a very good match upto 2 decimal places with the exact energy.The python notebook used for simulation can be found at this link.

4.3 Qubit Tapering using Symmetries

As prescribed in section (3) we use the symmetry of molecule Hamiltonian and use them to taper off the maximum no. of qubits (it includes the two qubit reduction also). The exact implementation is out of the scope for this work. However, we use the 'QML' package and its VQE solver to identify the symmetries and the relevant qubits tapered off. We reduce the no. of qubits from 12 to 8 by tapering off 4 qubits in the standard STO-3G basis. However, the precision is lost in this procedure, though the ground state energy remains same almost. However, the numerical values for pennylane's QMl library do not exactly match with that of Qiskit's. The exact ground state energy for interatomic distance with 1.55 Angstrom is approximately -7.66 Ha in the QML library. After tapering off the qubits, the ground state energy is same as -7.66 Ha. The python note book where results can be

checked can be found at this link.

5 Conclusion

From our work, we can see that Parity mapping is an excellent method to simulate ground state energy of molecules using VQE. The two qubit reduction method is further enhanced version of parity mapping with two qubits tapered such that the results almost match with the exact values. Further, we can use the point group symmetries to taper off more operators thereby, taper off more qubits for requiring the less no. of qubits for simulation, at very nominal loss of precision.

References

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