

Experimental exploration of virtual quantum subspace expansion using Qiskit

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Video at:
<https://youtu.be/23iXkLDLIG0>

Introduction

Molecular simulation is a promising candidate as the killer-application for near-term Noisy Intermediate-Scale Quantum (NISQ) technology. Research into efficient and accurate algorithms for molecular simulation in quantum computers has resulted in a continuous stream of techniques and enhancements, seeking to exploit the increased capacity of upcoming hardware [#cao2019quantum].

Since the introduction of the variational quantum eigensolver (VQE) in 2014 [#peruzzo2014variational], which signaled the possibility of performing molecular simulations on near-term quantum computers, there had been subsequent enhancements such as quantum subspace expansion (QSE)[#mcclean2017hybrid] and virtual quantum subspace expansion (VQSE) [#takeshita2020increasing], providing better approximations for energy bounds and the possibility of calculating excited states.

Molecule	Min	Max	Step
H_2	0.5	3	0.25
Li_2	2	10	0.5
LiH	2.5	4	0.25

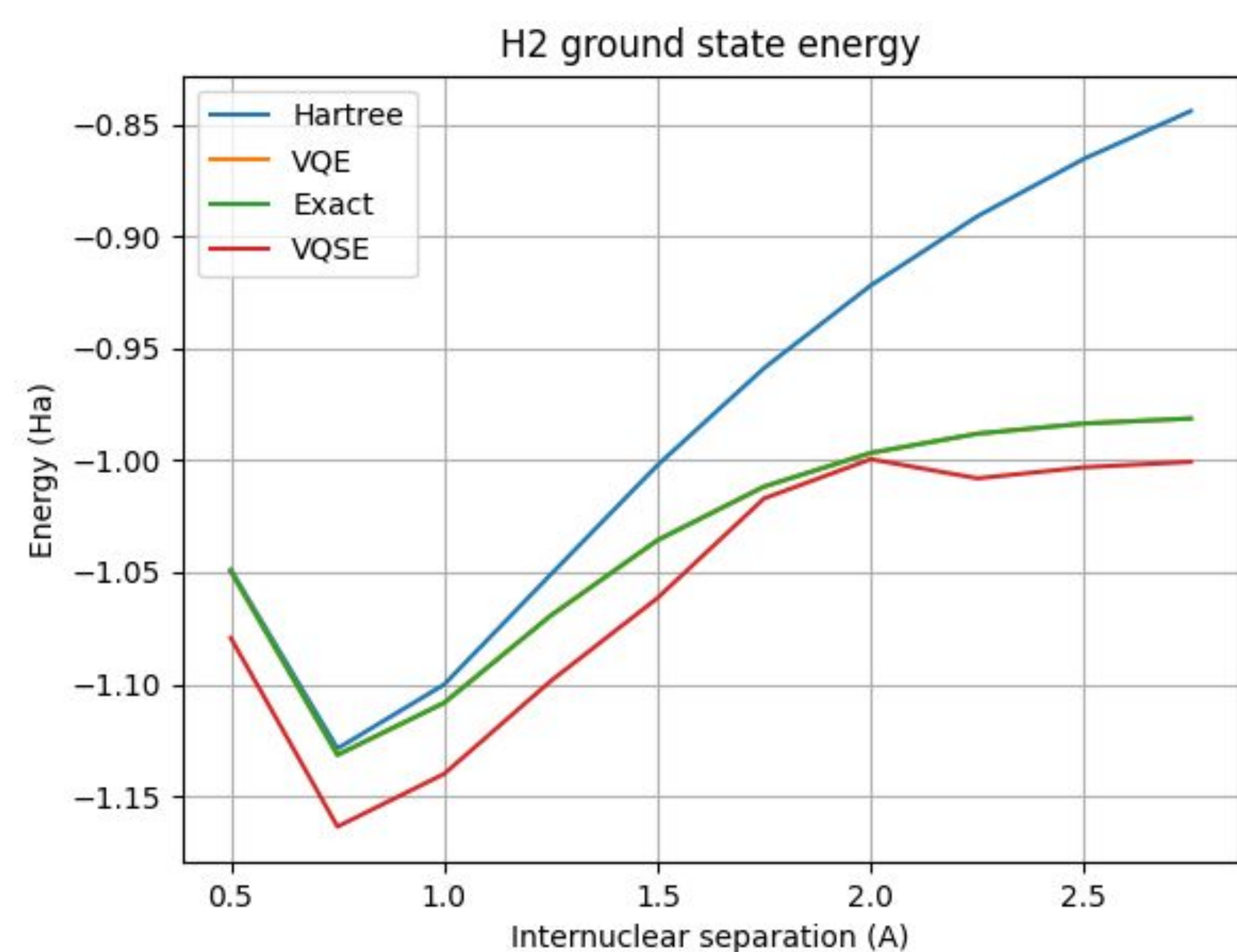
For experimentation purposes we selected three small molecules: H_2 , Li_2 , and LiH . These three molecules are usually found in molecular simulation tutorials and demonstrations; they are composed by two atoms and thus relatively easy to simulate and validate. For each of these molecules we determined a range of separation between atoms and expected minimum energies.

Method

The Virtual Quantum Subspace Expansion is a method for molecular simulation that improves on the Variational Quantum Eigensolver and Quantum Subspace Expansion, by performing additional classical calculations in order to enhance the predicted ground state energy. An initial Hartree-Fock state is used in a Variational Quantum Eigensolver subtask to approximate a ground state; VQE uses a Hamiltonian mapped from fermionic creation and annihilation operators, to be applied to a state ansatz which is optimized by exploiting the Rayleigh-Ritz variational formulation of the eigenvalue problem.

A common way of obtaining the Hamiltonian operator is using the Jordan-Wigner mapping, which represents fermionic creation and annihilation operators as sums of Pauli operators. This operator is parameterized according to which orbitals are core, active and virtual for particular applications. In the case of VQE only the active orbitals are taken into account.

VQSE perform corrections to the ground state by performing additional classical computations; this operators are defined for the combination of active and virtual orbitals. With this operators it defined an unrestricted Hamiltonian which is a projection in the ground state of the Hamiltonian on every pair of expansion operators



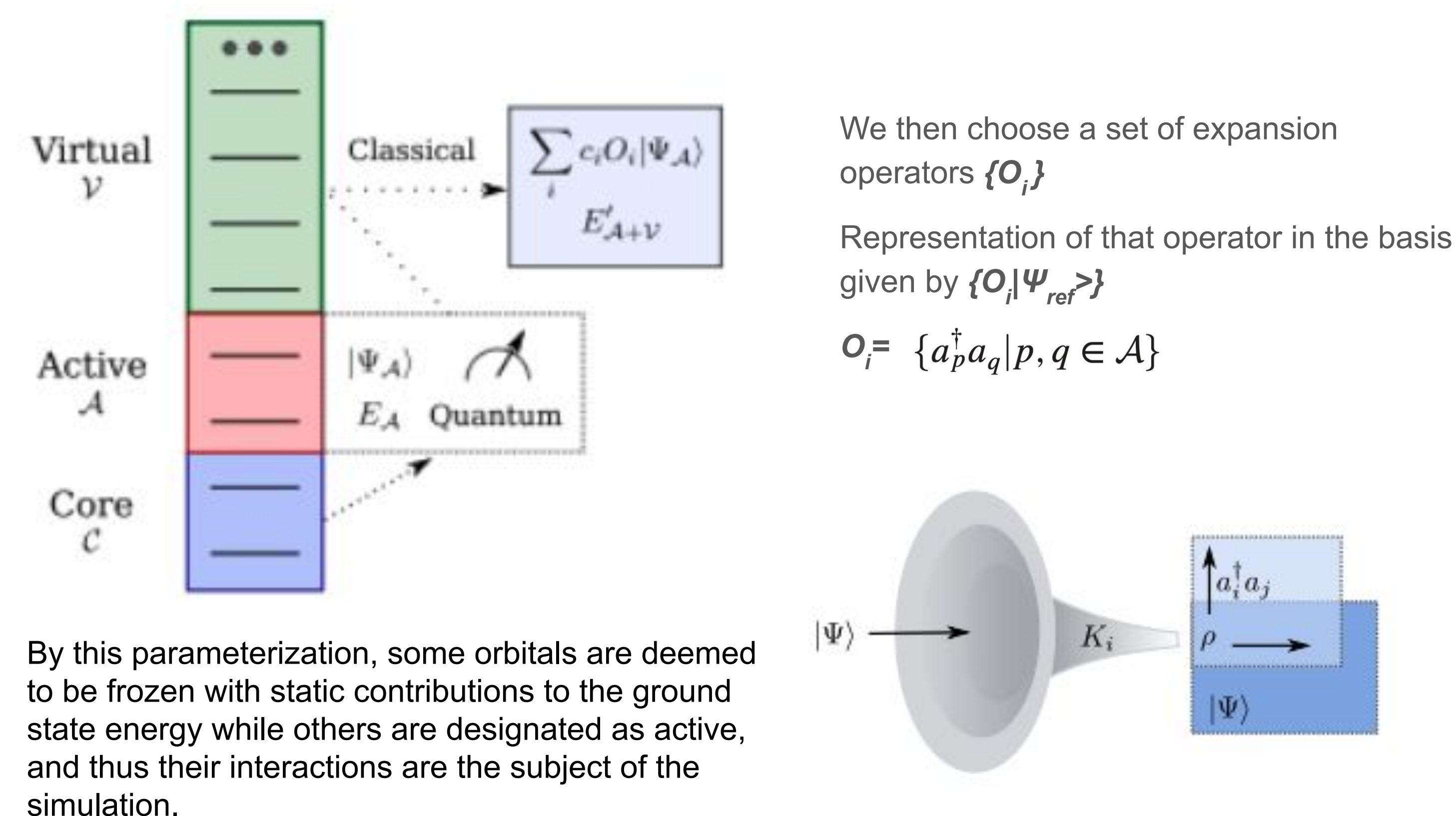
H_2 results. Since quantum computation was simulated, the VQE energies are hidden by the Exact energies. In this case we used no core orbitals, 2 active orbitals and 8 virtual orbitals.

Results & Discussion

The molecular parameters and active Hamiltonian operator calculation with the corresponding VQE evaluation execute immediately, even on online notebooks. We obtained 160, 134, and 134 expansion operators for H_2 , Li_2 , and LiH , respectively, which are also immediately calculated. The calculation of the unrestricted Hamiltonian operator takes less than 30s for each of the three molecules using FermiLib, but never finished in Qiskit.

The expectations on the ground state calculated for the evaluation of the unrestricted Hamiltonian and the overlap matrices are the bottleneck of the method. On initial implementations it did not finish for a single molecular separation after waiting for three days. After the parallel implementation the three molecules for a set of 36 separations took less than three hours. The generalized eigenvalue problem was calculated immediately.

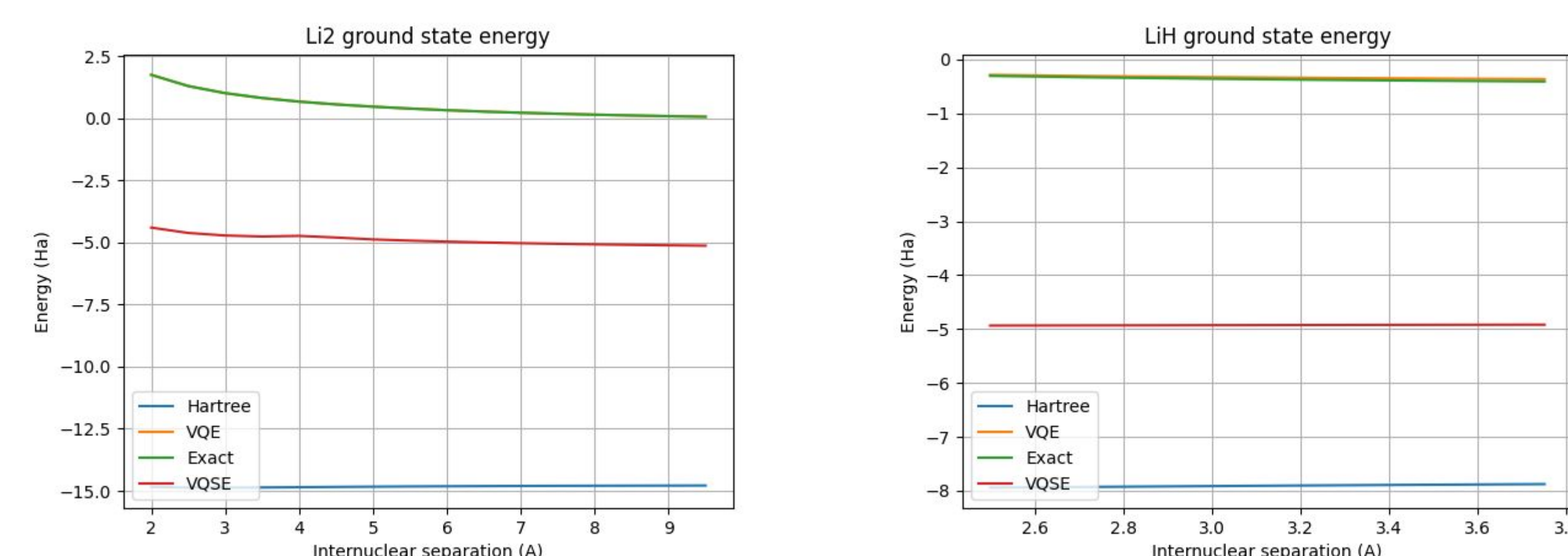
The results for Li_2 and LiH do not correspond to the reference values. There must exist an error in our implementation of core orbitals calculations. The reference energies for the simulations making use of core orbitals do not agree with our results.



By this parameterization, some orbitals are deemed to be frozen with static contributions to the ground state energy while others are designated as active, and thus their interactions are the subject of the simulation.

Conclusions

1. The evaluation of the unrestricted Hamiltonian and overlap matrices calculation are the bottleneck for VQSE molecule simulation. The necessary classical computational resources for VQSE were higher than we expected, it required specialized hardware. The required quantum resources for the evaluated molecules were minimal.
2. Further experiments with more complex molecules are required to validate the implementation. At the scale of the performed simulations it is not evident the break point in which molecular quantum simulation becomes an advantage. The current advances in molecular simulation algorithms using quantum computers suggest the possibility of more complex simulations when slightly more powerful quantum computers become available.
3. We implemented a recent method for molecular simulation. Although Qiskit is perhaps the most mature software package for quantum computing, there are still relevant use cases missing that increased the difficulty of this implementation.



(Left) Li_2 results. Since quantum computation was simulated, the VQE energies are hidden by the Exact energies. In this case we used 2 core orbitals, 2 active orbitals and 6 virtual orbitals. (Right) LiH results. Since quantum computation was simulated, the VQE energies are partially hidden by the Exact energies. In this case we used 1 core orbital, 2 active orbitals and 6 virtual orbitals.

References

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