Report: Entanglement entropy of Hydrogen molecule

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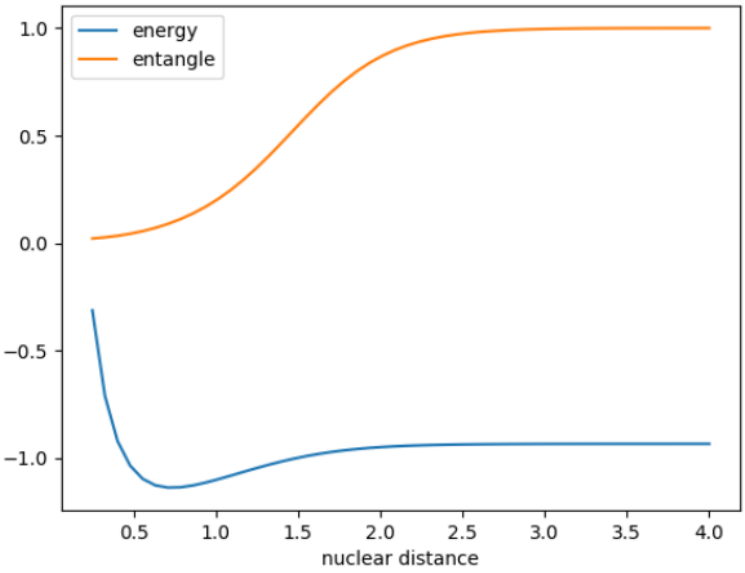
The Hydrogen molecule is consistent of two interacting Hydrogen atoms and we would like to get the entanglement between the two atoms. I have tried some methods to get the ground state and these gives me totally different results

1 direct decomposition

The terms in the molecular Hamiltonian can be viewed as a Pauli strings and also as a tensor products of some Pauli operators, so the Hamiltonian itself is a matrix of 2n dimension. then we can direct perform a eigen-decomposition on the matrix and for the 4-qubit Hamiltonian we'd like to take the first as atom A.

- In the OpenFermion package there exists function 0getsparseoperator0 and 'eigenspectrum' that can directly get the eigenvalue and eigenvector. The terms expect $|1100\rangle$ and $|0011\rangle$ are very small and we can take the resulting two terms, the result is shown:



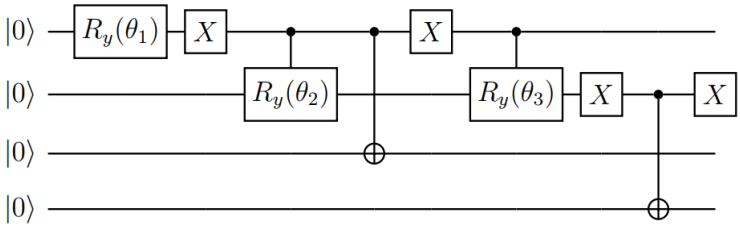
- Apart from the Openfermion we can directly transform the Hamiltonian into matrix and get the eigen-information. Compare with the result above, there difference in energy is at about 10^{-14}, but the corresponding eigenvector is a direct product state $|0110\rangle$, leading to a 0 of the entanglement entropy.

2 VQE

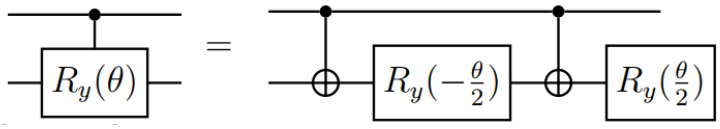
To compute the entanglement entropy of the Hydrogen molecule, first we use the ansate:

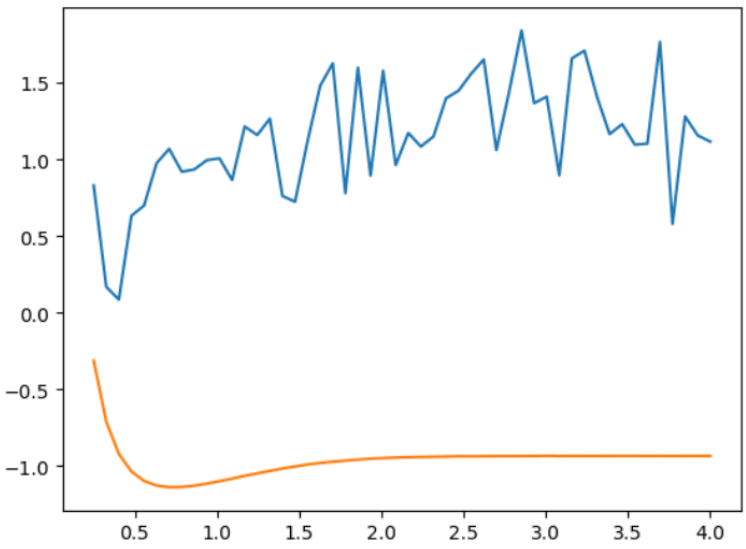
$|\psi\rangle = a|0011\rangle + b|0101\rangle + c|1001\rangle + d|1100\rangle$

We use the following quantum circuit to prepare the state



where: and the result is:





3 Discussion

There are some reasons leading to this difference:

- The intractable problem is to know hoe the electron and orbitals are encoded to the qubit form and thus for the state $|q_0q_1q_2q_3\rangle$, we don't know each qubit represents
- In the OpenFermion it is said to be molecular orbitals and therefore we direct think the first two qubits as atom A is not proper.
- The VQE approach has a bad overlap with the eigenvalue, which may be caused by the optimization process. Because the main idea is to get the energy but not the state.