Computational Quantum Physics
Exercise 14

PHYS-463
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Problem 14.1 The variational quantum eigensolver

In this exercise we want to use the Variational Quantum Eigensolver (VQE) algorithm to prepare a variational approximation of the ground state of the H_2 molecule at different bond-lengths d and study its dissociation process.

a) Follow the tutorial to see how the second quantization fermionic Hamiltonian produced by PySCF can be mapped into a linear combination of Pauli strings that can be measured on a quantum device using Qiskit.

b) In this mapping, prepare the initial state corresponding to the Hartee-Fock approximation of the ground state. Then, define a variational circuit that will be applied to this initial state. Keep in mind that the shallower the circuit the lesser it will be affected by noise in a real simulation.

c) Create a function to measure the expectation value of the fermionic operator and its derivatives with respect to the variational parameters.

d) Perform the optimization on the equilibrium configuration of H_2 ($d_{H_2} = 0.735\,\text{Å}$) using the STO-6G basis, are you able to reach the FCI energy in this case?

e) Finally, perform the VQE on the H_2 system at different bond-lengths d and compare the results with the HF, FCI and CCSD methods explored in previous lectures.