ISSUE #37: VQE FOR PARTICLE-CONSERVING HAMILTONIAN

- Consider a fermionic system described by the hamiltonian

$$H = \sum_{p,q} h_{pq} a_p^+ a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^+ a_q^+ a_r a_s$$

- In general circuit wave-functions don't conserve the number of particles of the system → Add a particle-number-conserving constraint c to H to get: $H' = H + c$

$$c = \alpha\left(\sum_{i=0}^{n-1} a_i^+ a_i - N\right)^2$$

  α is a parameter and N is the total number of the particles

- Use the VQE algorithm in Qiskit Aqua on H' and evaluate $\langle E \rangle = \langle \psi | H | \psi \rangle$ with the optimized wave function ψ
- Modified Modules:

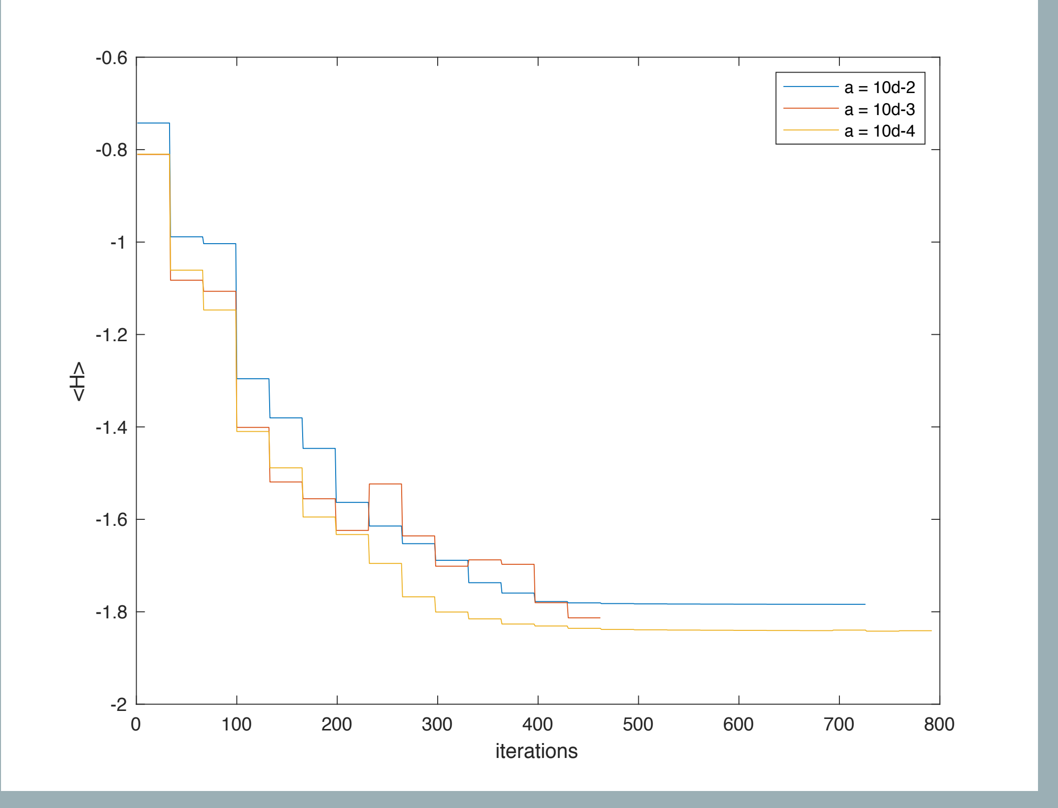
  qiskit.chemistry.FermionicOperator (to add the constraint)

  qiskit.chemistry.EnergyEvaluation (to calculate $\langle E \rangle$)

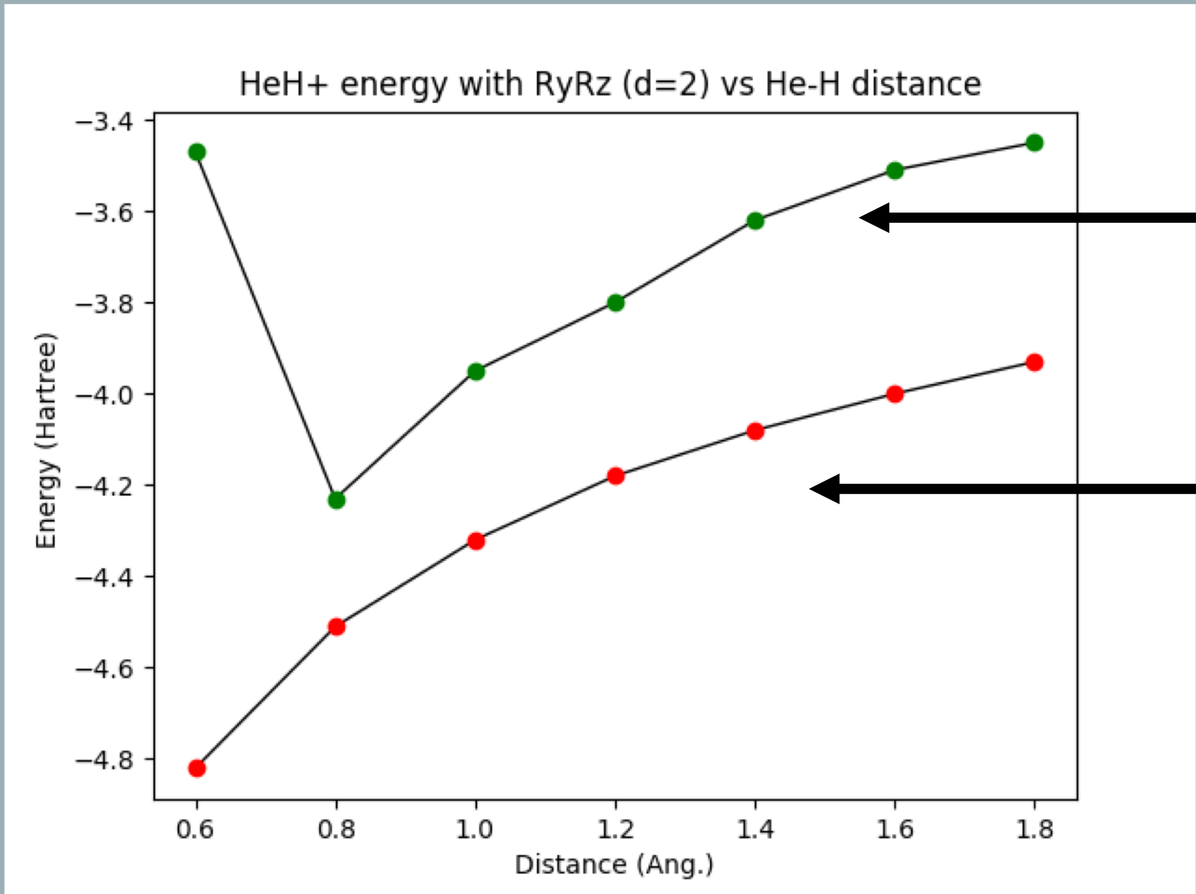
  other modules connected to those

$$c = \alpha\left(\sum_p a_p^+ a_p - N\right)^2 = \alpha N^2 - 2N\alpha \sum_p a_p^+ a_p + \alpha \sum_{p,q} a_p^+ a_p a_q^+ a_q$$

Plot: H_2, basis:STO3g, mapping: Jordan-Wigner for different values of α



Plot: HeH^+ energy , basis: 6-31g, mapping: Jordan-Wigner, $\alpha = 1$



With Constraint
(2 electrons HeH^+)

Without constraint
(3 electrons HeH)