pHw6

Wednesday, April 27, 2022 3:39 PM

Problem Set 6

AS.171.402: Applied Quantum Information [Spring 2022]

Due Date: May 1, 2022 (11:59 pm)

Simulating the ground state of the Hydrogen Molecule using VQE

In this problem set, we will explore the use of the Variational Quantum Eigensolver (VQE) algorithms to simulate and identify the ground state of the Hydrogen molecule.

The hydrogen molecule, H_2, consists of two-electrons, and in a minimal basis representation each electron has orbital and spin degrees of freedom. Therefore, the energy of the molecule can be modeled using a Hamiltonian on two qubits. Quantum information theorists in collaboration with quantum chemists have mapped the minimal Hamiltonian on to one acting on two-qubits,

$$\hat{H} = g_0 + g_1\hat{Z}_1 + g_2\hat{Z}_2 + g_3\hat{Z}_1\hat{Z}_2 + g_4\hat{Y}_1\hat{Y}_2 + g_5\hat{X}_1\hat{X}_2, \tag{1}$$

where, the parameters $\{g_0, g_1 \cdots g_5\}$ are scalar parameters that are dependent on the bond length, R of the molecule.

In this problem, we will try to reproduce the following ground-state energy dependence of the Hydrogen molecule on bond-length R using the VQE algorithm.

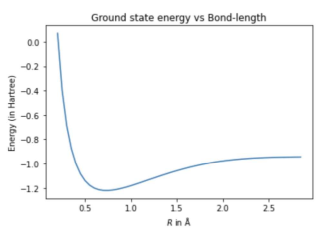


FIG. 1: Ground state energy dependence on the bond-length of the Hydrogen molecule.

We provide an accompanying dataset `g_values.csv` that contains the values of g_j,

$j \in \{0, \cdots, 5\}$ for increasing R. In the following, we will use the Variational Quantum Eigensolver (VQE) algorithm to solve for the ground state of the Hamiltonian shown in Eq. 1.

(a) We start by constructing a variational circuit ansatz based on known physics of the molecule. The ansatz wavefunction for the ground state based on Hartree-Fock theory and the Unitary Coupled Cluster Theory is given by,

$$|\psi_{\rm UCC}(\Theta)\rangle = e^{-i\Theta\hat{Y}_1\hat{X}_2}\,|10\rangle\,. \tag{2}$$

where $\Theta \in [0, 2\pi)$ is the variational parameter to be optimized over.

(i) Show that $e^{-i\Theta\hat{Y}_1\hat{X}_2} = \hat{V}^\dagger\, e^{-i\Theta\hat{Z}_1\hat{Z}_2}\,\hat{V}$, with $\hat{V} = R_x\left(-\frac{\pi}{2}\right) \otimes R_y\left(\frac{\pi}{2}\right)$.

(ii) Construct a two-qubit circuit that prepares the variational state $|\psi_{\rm UCC}(\Theta)\rangle$ using only the following gates: $\{\hat{R}_x(\theta), \hat{R}_y(\theta), \hat{R}_z(\theta), \hat{CX}\}$.

[Hint: Use the decomposition of the gate $R_{zz}(\theta) = e^{-i\frac{\theta}{2}\hat{Z}_1\hat{Z}_2}$ in terms of two $\hat{CX}$ gates.]

(ii) In the accompanying jupyter notebook, write a function `create_UCC_ansatz(theta)` that returns a parametrized circuit the as obtained in (ii).

(iii) Calculate analytically the expectation value of the Hamiltonian in Eq. 1 as a function of Θ.

[Hint: Expand the exponential in Eq. 2 and simplify.]

$Y|0\rangle = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ i \end{bmatrix}$

$Y|1\rangle = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -i \\ 0 \end{bmatrix}$

a) i) $e^{-i\theta\hat{Y}_1\hat{X}_2} = \hat{V}^\dagger e^{-i\theta Z_1 Z_2}\hat{V}$ $R^\dagger(\theta) = R(-\theta)$ $V^\dagger e^A V = e^{V^\dagger A V}$

$= e^{\hat{V}^\dagger -i\theta Z_1 Z_2 \hat{V}}$

$R_x(\frac{\pi}{2}) Z R_x(-\frac{\pi}{2}) = \hat{Y}_1$

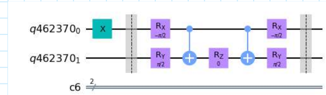
$R_y(\frac{-\pi}{2}) Z R_y(\frac{\pi}{2}) = \hat{X}$

$= e^{-i\theta (R_x(\frac{\pi}{2}) \otimes R_y(-\frac{\pi}{2}))(Z_1 \otimes Z_2)(R_x(-\frac{\pi}{2}) \otimes R_y(\frac{\pi}{2}))}$

$= e^{-i\theta (R_x(\frac{\pi}{2})\hat{Z}_1 \otimes R_y(\frac{\pi}{2})\hat{Z}_2)(R_x(-\frac{\pi}{2}) \otimes R_y(\frac{\pi}{2}))}$

$= e^{-i\theta \hat{Y}_1 \otimes \hat{X}_2}$

ii)



iii) $\langle\psi|\hat{H}|\psi\rangle = \langle\psi| g_0 + g_1\hat{Z}_1 + g_2\hat{Z}_2 + g_3\hat{Z}_1\hat{Z}_2 + g_4\hat{Y}_1\hat{Y}_2 + g_5\hat{X}_1\hat{X}_2 |\psi\rangle$

(distribute)

$e^{-i\theta\hat{Y}_1\hat{X}_2} = \cos(\theta)I - i\sin(\theta)\hat{Y}_1\hat{X}_2 \xrightarrow{|10\rangle} = \cos(\theta)|10\rangle - i\sin(\theta)\cdot -i|01\rangle$

$|\psi\rangle = \cos(\theta)|10\rangle - \sin(\theta)|01\rangle$

$\langle\psi|g_0|\psi\rangle = \langle 10| e^{i\theta\hat{Y}_1\hat{X}_2}\; g_0\; e^{-i\theta\hat{Y}_1\hat{X}_2}|10\rangle$

$= [\langle 10|\cos(\theta) + \sin(\theta)\langle 01|]\, g_0 [\cos(\theta)|10\rangle - \sin(\theta)|01\rangle]$

$= g_0 [\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta)\underbrace{\langle 10|01\rangle}_{0} - \cos(\theta)\sin(\theta)\underbrace{\langle 01|10\rangle}_{0} + \sin^2(\theta)\langle 01|01\rangle]$

$= g_0 [\cos^2(\theta) + \sin^2(\theta)]$

$= g_0$

$\langle\psi| g_1\hat{Z}_1|\psi\rangle = g_1\hat{Z}_1[\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta)\langle 10|01\rangle - \cos(\theta)\sin(\theta)\langle 01|10\rangle + \sin^2(\theta)\langle 01|01\rangle]$

$= g_1[\cos^2(\theta)\cdot -\langle 10|10\rangle + \cos(\theta)\sin(\theta)\langle 10|01\rangle - \cos(\theta)\sin(\theta) - \langle 01|10\rangle + \sin^2(\theta)\langle 01|01\rangle]$

$= g_1[\sin^2(\theta) - \cos^2(\theta)] = -g_1\cos(2\theta)$

$\langle\psi| g_2\hat{Z}_2|\psi\rangle = g_2\hat{Z}_2[\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta)\langle 10|01\rangle - \cos(\theta)\sin(\theta)\langle 01|10\rangle + \sin^2(\theta)\langle 01|01\rangle]$

$= g_2[\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta) - \langle 10|01\rangle - \cos(\theta)\sin(\theta)\langle 01|10\rangle + \sin^2(\theta) - \langle 01|01\rangle]$

$= g_2[\cos^2(\theta) - \sin^2(\theta)] = g_2\cos(2\theta)$

obtained in (ii).

(iii) Calculate analytically the expectation value of the Hamiltonian in Eq. 1 as a function of Θ.

$Y|0\rangle = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ i \end{bmatrix}$

$Y|1\rangle = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -i \\ 0 \end{bmatrix}$

[Hint: Expand the exponential in Eq. 2 and simplify.]

(iv) Using the expression for the expectation value in part (iii), and elementary calculus, obtain the analytical expression for Θ in terms of the parameters g_j that minimizes the expectation value.

(c) Having defined a circuit to generate the ansatz, next we set up the necessary measurements to implement a VQE algorithm. Show that measuring all qubits along x, y and z is sufficient to calculate the expectation value of the Hamiltonian. Implement these circuits in `measurement_circuits()` in the accompanying jupyter notebook. We have provided a function, `calculate_expectation_value()` that computes the expectation value of the provided Hamiltonian from the measurement outcomes.

$= g_1 [\sin^2(\theta) - \cos^2(\theta)] = -g_1 \cos(2\theta)$

$\langle\psi| g_2 \hat{z}_2 |\psi\rangle = g_2 \hat{z}_2 [\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta)\langle 10|01\rangle - \cos(\theta)\sin(\theta)\langle 01|10\rangle + \sin^2(\theta)\langle 01|01\rangle]$

$= g_2 [\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta) - \langle 10|01\rangle - \cos(\theta)\sin(\theta)\langle 01|10\rangle + \sin^2(\theta) - \langle 01|01\rangle]$

$= g_2 [\cos^2(\theta) - \sin^2(\theta)] = g_2 \cos(2\theta)$

$\langle\psi| g_3 \hat{z}_1 \hat{z}_2 |\psi\rangle = g_3 \hat{z}_1 \hat{z}_2 [\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta)\langle 10|01\rangle - \cos(\theta)\sin(\theta)\langle 01|10\rangle + \sin^2(\theta)\langle 01|01\rangle]$

$= g_3 [\cos^2(\theta) - \langle 10|10\rangle + \cos(\theta)\sin(\theta) - \langle 10|01\rangle - \cos(\theta)\sin(\theta) - \langle 01|10\rangle + \sin^2(\theta) - \langle 01|01\rangle]$

$= g_3 [-\cos^2(\theta) - \sin^2(\theta)] = -g_3$

$\langle\psi| g_4 \hat{Y}_1 \hat{Y}_2 |\psi\rangle = g_4 \hat{Y}_1 \hat{Y}_2 [\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta)\langle 10|01\rangle - \cos(\theta)\sin(\theta)\langle 01|10\rangle + \sin^2(\theta)\langle 01|01\rangle]$

$= g_4 [\cos^2(\theta) - i^2\langle 10|01\rangle + \cos(\theta)\sin(\theta) - i^2\langle 10|10\rangle - \cos(\theta)\sin(\theta) - i^2\langle 01|01\rangle + \sin^2(\theta) - i^2\langle 01|10\rangle]$

$= g_4 [\cos(\theta)\sin(\theta) + \cos(\theta)\sin(\theta)]$

$\langle\psi| g_5 \hat{x}_1 \hat{x}_2 |\psi\rangle = g_5 \hat{x}_1 \hat{x}_2 [\cos^2(\theta)\langle 10|10\rangle + \cos(\theta)\sin(\theta)\langle 10|01\rangle - \cos(\theta)\sin(\theta)\langle 01|10\rangle + \sin^2(\theta)\langle 01|01\rangle]$

$= g_5 [\cos^2(\theta)\langle 10|01\rangle + \cos(\theta)\sin(\theta)\langle 10|10\rangle - \cos(\theta)\sin(\theta)\langle 01|01\rangle + \sin^2(\theta)\langle 01|10\rangle]$

$= g_5 [\cos(\theta)\sin(\theta) + \cos(\theta)\sin(\theta)]$

$\langle\psi|H|\psi\rangle = g_0 + \cos(2\theta)(g_2 - g_1) - g_3 - \sin(2\theta)(g_4 + g_5)$

iv) $\langle\psi|H|\psi\rangle = \underbrace{(g_0 - g_3)}_{\text{Constant}} + \underbrace{\cos(2\theta)}_{\text{depends on}}(g_2 - g_1) - \sin(2\theta)(g_4 + g_5)$

$\frac{d}{d\theta}\langle\psi|H|\psi\rangle = -2(g_2 - g_1)\sin(2\theta) - 2(g_4 + g_5)\cos(2\theta)$

min $= 0 \Rightarrow (g_2 - g_1)\sin(2\theta) = -(g_4 + g_5)\cos(2\theta)$

$\tan(2\theta) = \frac{-(g_4 + g_5)}{(g_2 - g_1)}$

$\theta = \tan^{-1}\left(\frac{-(g_4 + g_5)}{(g_2 - g_1)}\right)/2$

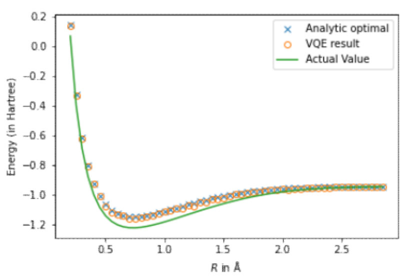
(d) Next, we would like to find numerically the optimal value of Θ for a given set of parameters $\{g_j\}$. Since the ansatz depends on only one parameter, we can use exhaustive search to find the solution. In the accompanying jupyter notebook, define a function `exhaustive_search()`, that calculates the expectation value of the Hamiltonian for a 100 different values of Θ (noting that $0 \leq \Theta < 2\pi$) and identifies the optimal value of Θ by searching for the minimum angle.

(e) Finally, using the exhaustive search function, obtain the optimal value of the ground state energy for each set of parameters, and compare against the data in Fig. 1 and the analytical solution obtained in part (a).

c)

d) done

e)



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