

## ME 201/APh 250, Homework 4:

Assigned: Wednesday, May 1, 2019

Due: Wednesday, May 15, 2019

1. For the first part of this assignment, you will be applying the Jordan-Wigner(JW) transformation to map the Hamiltonian that describes the hydrogen molecule in the occupation number basis to spin operators.

Suppose we construct the Hamiltonian of hydrogen molecule in the occupation basis set using the chemical basis STO-6G. The electrons will occupy four spin-orbitals (two spatial components and two spin components). We labelled them as  $|\chi_i\rangle$ ,  $i = 1,2,3,4$ . The electronic structure Hamiltonian in the occupation number basis for molecular orbitals is:

$$H = H^{(1)} + H^{(2)} \quad (1)$$

$$H^{(1)} = \sum_{p=0}^3 h_{pp} a_p^\dagger a_p \quad (2)$$

$$H^{(2)} = h_{0110} a_0^\dagger a_1^\dagger a_1 a_0 + h_{2332} a_2^\dagger a_3^\dagger a_3 a_2 + h_{0330} a_0^\dagger a_3^\dagger a_3 a_0 + h_{1221} a_1^\dagger a_2^\dagger a_2 a_1 + \quad (3)$$

$$(h_{0220} - h_{0202}) a_0^\dagger a_2^\dagger a_2 a_0 + (h_{1331} - h_{1313}) a_1^\dagger a_3^\dagger a_3 a_1 +$$

$$h_{0312} (a_0^\dagger a_3^\dagger a_1 a_2 + a_2^\dagger a_1^\dagger a_3 a_0) +$$

$$h_{0132} (a_0^\dagger a_3^\dagger a_1 a_2 + a_2^\dagger a_3^\dagger a_1 a_0)$$

From this Hamiltonian we see there are a few classes of terms: (1) the one-electron terms; (2) terms of the form  $a_0^\dagger a_1^\dagger a_1 a_0$ ; (3) terms like  $(a_0^\dagger a_3^\dagger a_1 a_2 + a_2^\dagger a_1^\dagger a_3 a_0)$ . Using certain values for  $h_{pq}$  and  $h_{pqrs}$ , Seeley and co-workers[1] had worked out the JW transformation to be :

$$H^{(JW)} = - 0.812611 + 0.171201\sigma_0^z + 0.171201\sigma_1^z - 0.2227965\sigma_2^z - 0.2227965\sigma_3^z \quad (4)$$

$$+ 0.16862325\sigma_1^z\sigma_0^z + 0.12054625\sigma_2^z\sigma_0^z + 0.1658680\sigma_2^z\sigma_1^z + 0.1658680\sigma_3^z\sigma_0^z$$

$$+ 0.12054625\sigma_3^z\sigma_1^z + 0.17434925\sigma_3^z\sigma_2^z$$

$$- 0.04532175\sigma_3^x\sigma_2^x\sigma_1^y\sigma_0^y + 0.04532175\sigma_3^x\sigma_2^y\sigma_1^y\sigma_0^x$$

$$+ 0.04532175\sigma_3^y\sigma_2^x\sigma_1^x\sigma_0^y - 0.04532175\sigma_3^y\sigma_2^y\sigma_1^x\sigma_0^x$$

(a) Using the coefficients from table III in [1], verify the JW transform Seeley obtained. Split your solution into two parts:

(i) Use the JW transformation for terms belonging to classes of terms in (1) and (2). These provide the first three lines of equation 4 [10 marks].

(ii) The JW transform of the remaining terms will give the last 2 lines of equation 4 [2 marks].

(b) Draw the circuits that would implement a single Trotter step  $e^{-i\hat{H}}$  (meaning sums of terms in an exponential are approximated as sequential applications of exponentials of each term) [3 marks]. This provides a way for one to perform phase estimation to try and obtain the ground state.

2. The JW transform we verified earlier indicates that one might need to use 4-qubits to carry out the calculations. By symmetry arguments, it was realized that the Hamiltonian in the Bravyi-Kitaev basis can be reduced into a 2-qubit form:

$$\hat{H} = g_0(R)\mathbf{I} + g_1(R)\sigma_0^z + g_2(R)\sigma_1^z + g_3(R)\sigma_0^z\sigma_1^z + g_4(R)\sigma_0^x\sigma_1^x + g_5(R)\sigma_0^y\sigma_1^y \quad (5)$$

The coefficients depend on the inter-atomic distance between the hydrogen atoms. Using the single parameter UCC ansatz:

$$|\phi(\theta)\rangle = e^{-i\theta/2X_0Y_1} |01\rangle \quad (6)$$

O'Malley and co-workers obtained the electronic structure of the hydrogen molecule using variational quantum eigensolver(VQE)[2]. Let's us try to reproduce the potential energy surface curve using VQE:

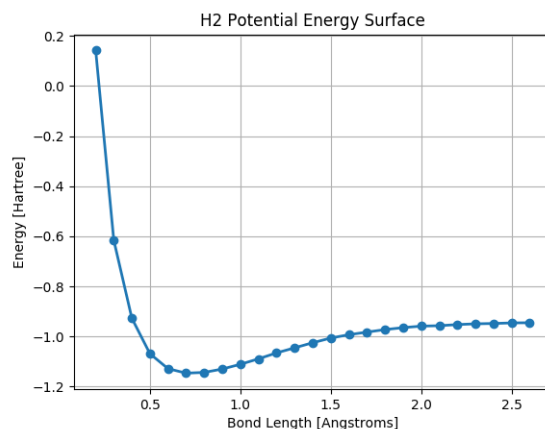


Figure 1: Potential energy surface of hydrogen molecule using VQE.

It will be useful to go through the Jupyter notebook that explains how one goes about implementing VQE. The required coefficients are also provided in a data file *vqe.dat*. For this problem, always start with an initial guess of  $\theta = 0.0$ .

(a) Plot the optimization trajectories obtained using the method Nelder-Mead and Powell for  $R = 0.2\text{\AA}$  on the same graph. Do the same for  $R = 0.6\text{\AA}$ . Comment on the relative performance of the different optimizer [5 marks].

(b) Perform VQE to obtain the potential energy surface like the ones given above [10 marks].

1. J.T. Seeley, M.J. Richard, and P.J. Love. J. Chem. Phys. **137**, 224109 (2012).
2. P.J.J. O'Malley et. al. Phys. Rev. X **6**, 031007 (2016).