Simulating the Water Molecule using a Quantum Walk algorithm

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March 1, 2020

Abstract

bla

1 Introduction

Why would we do this

[**test**] [**bla**]

3 % of the world's energy output is spent on making fertilizer [**femoco**]. We currently rely on a highly outdated, energy intensive process requiring very large amounts of natural gas. There is an anaerobic bacteria however perfoming the very same process while requiring much less energy, utilizing nitrogen fixation with molecules such as FeMoCo. Traditional chemical analyses have not been able to give us an understanding on the details of this process, and as this molecule is highly complex, simulations using classical supercomputers are out of reach. Reiher et al. have shown that quantum computers

It can be done

Expand more on quantum chemistry, why quantum computers have the edge over classical Common methods are Trotter-suzuki: Second quantized Hamiltonian

Importance of error correction?
How has it so far been done
How am i going to do it
[**quantumwalk**]

2 Research Context

Expand on the multiple other methods (VQE)

"To obtain the Hamiltonian of the water molecule, we start by considering the 1s orbital of each hydrogen atom along with the 1s, 2s, 2px, 2py, 2pz orbitals for the oxygen atom. This leads to a total of 14 molecular orbitals considering spin. To make our simulations more efficient, the number of qubits is reduced by considering orbital energies and exploiting the symmetry of the system [22]. It can be initially assumed that the two molecular orbitals of largest energies are unoccupied. Consequently, the calculation of the Hamiltonian of the water molecule then only requires the consideration of 12 spin-orbitals. After second quantization, the Hamiltonian can be expressed as [23]:"

With The second quantized Hamiltonian of the static water molecule generally has the form:

$$H = \sum_{i,j=1}^{12} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{12} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

In this Hamiltonian, $a_i^\dagger$ and a_j are the fermionic annihiliation and creation operators and h is the respective interaction coefficient. Biang et al. reduce this Hamiltonian to the following form, using parity transformations and simplifications to the following form:

$$H = \sum_{i=j}^{N} \alpha_j P_j$$

Here, α_j is a propagating? coefficient, and P_j is some tensor product of the four Pauli operators, defined as the following:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The Hamiltonian sums up to N terms, where $N = 2^4 = 16$, equal to the number of possible multi-qubit operators.

Biang et al. compare five methods for calculating the ground-state energy of the water molecule, namely:

- *Trotter Phase Estimation Algorithm*
  This method uses Trotter-Suzuki decompositio(n to approximate the propagating term $e^{-i\alpha_i h_i t}$, and subsequently extracts the ground state energy from the phase. The Trotter PEA requires $\mathcal{O}(n)$ qubits to run and has a gate complexity of $\mathcal{O}(\left(\frac{n^5}{(\epsilon/A)^2}\right))$

- *Direct Implementation of Hamiltonian in First Order*
  This method largely relies on the same principles as the Trotter PEA, but it employs a different unitary operator U. This Direct-PEA requires $\mathcal{O}(n)$ qubits to run and has a gate complexity of $\mathcal{O}(\left(\frac{n^5}{(\epsilon/A)^2}\right))$
- *Direct Implementation of Hamiltonian in Second Order*
  This method is the same as the First Order Direct-PEA, but it approximates U to the second order instead. This variant of the Direct-PEA requires $\mathcal{O}(n)$ qubits to run and has a gate complexity of $\mathcal{O}(\left(\frac{n^5}{(\epsilon/A)^{1.3}}\right))$
- *Direct Measurement of Hamiltonian*
  This method translates the Hamiltonian directly into a quantum circuit and retrieves the ground energy by repeatedly measuring. Direct measurement requires $\mathcal{O}(n)$ qubits to run and has a gate complexity of $\mathcal{O}(\left(n^5\right))$
- *Variational Quantum Eigensolver*
  The VQE prepares a trial wave function and approximates the energy by iteratively retrieving the Pauli operator tensor products. This algorithm

3 Methodology

Cirq

4 Writing Update

Method	Qubits Requirement	Gate Complexity
Trotter-PEA	$O(n)$	$O\left(\frac{n^5}{(\epsilon/A)^2}\right)$
Direct-PEA $\left(1^{st}\text{ order }\right)$	$O(n)$	$O\left(\frac{n^5}{(\epsilon/A)^{2.5}}\right)$
Direct-PEA $\left(2^{nd}\text{ order }\right)$	$O(n)$	$O\left(\frac{n^5}{(\epsilon/A)^{1.3}}\right)$
Direct Measurement	$O(n)$	$O\left(n^5\right)$
Pairwise VQE	n	$O\left(n^2 d\right)$