Quantum Simulation of the H_2 Molecule*

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ABSTRACT

Our project focuses on simulating the behavior and energy of the H2 molecule in various quantum scenarios. Through this exploration, we've captured key insights into the ground state energy and effects of different perturbations.

l Simulation and Ground State
- H2 Molecule: Simulated the H2 molecule using a quantum approach.
- VQE (Variational Quantum Eigensolver): Determined the ground state energy of the H2 molecule.

Trotterisation and Perturbation
- Trotterisation: Applied the Trotterisation method to see the changes in energy due to a perturbation.
- Time-Dependent Perturbation: Introduced a time-dependent perturbation to study its effects.

Application of Magnetic Field
- Magnetic Field Orientation: Applied a magnetic field that transitions from the X to the Z axis.
- Analysis: Observed and documented the effect of the changing magnetic field on the ground state energy of the H2 molecule.

I. INITIAL SIMULATION AND GROUND STATE H2 MOLECULE

A. Simulated the H2 molecule

We utilized Qiskit's 'PySCFDriver'' to define the H_2 molecule. The electronic structure of the molecule is initially described in terms of fermionic creation and annihilation operators.

Now, transform this fermionic Hamiltonian into a qubit (spin) Hamiltonian suitable for quantum computation. For our simulation we have used Jordan-Wigner Transformation which provides a direct mapping of fermions to qubits. Bravyi-Kitaev Transformation is another more efficient mapping especially for systems with local interactions, but its more complex in form.

B. VQE (Variational Quantum Eigensolver)

Now, we can use Variational Quantum Eigensolver(VQE) to determine the ground state of the hydrogen atom.

For this we used 'TwoLocal'' ansatz in Qiskit. It is is a quantum circuit template used in VQE, and alternates between R_y and C_Z gates We used this structure since it provides a balance between expressiveness and computational efficiency, making it a popular choice for approximating quantum states.

II. EVOLUTION OF H2 MOLECULE

Now, to find the time evolution of H2 molecule, we can use a couple of approaches:

1. Time evolution by matrix exponentation(Naive): We can multiply the Hamiltonians at small dt intervals. However, its a complex process
2. Trotterisation: It helps to approximate the Hamiltonian, thereby making it more computationally efficient.
3. Magnus Expansion: Another way to approximate a Time dependent Hamiltonian

A. Use to find the time evolution

We utilized Qiskit's 'SuzukiTrotter' to evolve the H_2 molecule in time.

For this we first used a time independant Hamiltonian and first order Trotterisation, and we observe that Trotterisation matches the exact energy.

Next, we apply $H_{\text{perturbation}}$ as stated below, to see how well Trotterisation is able to approximate the time evolution of Hamiltonian.

$$H_{\text{perturbation}} = -h\left(\sum_{i=0}^{N-1} \sin(\alpha)Z_i + \cos(\alpha)X_i\right)$$

We observe that for first order Trotterisation, the variations are significant. But as we increase the order, from $1 \to 2 \to 4$, the accuracy energy evolution fit gets better.

* A footnote to the article title