Quantum Simulation of the H_2 Molecule

Roberto Negrin, Saleh Naghdi, Yarin Heffes, and Manvi Agrawal

University of California, Los Angeles, California

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Our project focuses on simulating the behavior and energy of the H_2 molecule in various quantum scenarios. We used Trotterisation to evaluate the time evolution of the Hydrogen molecule by itself, and then its response to a static perturbation such as that induced by an external magnetic field. We further extended our investigation to the case of a time-varying perturbation where the Hydrogen molecule is exposed to a time-dependent external magnetic field. The jump from analysing static to changing perturbations was not trivial, however. In the case of a time-dependent Hamiltonian the evolution operator can no longer be expressed as a matrix exponential which is the required form for Trotterisation. Instead, we employed a Riemann-Sum approach, discretizing our time-dependent Hamiltonian into many small intervals and then applying Trotterization within each interval. For our final foray, we utilized this technique to demonstrate the famous adiabatic principle in quantum mechanics which forms the basis of adiabatic quantum computing.

I Project Choice Explanation

We, as MQST master's students with a robust foundation in both physics and computer science, bring to the table an advanced QIS experience level 4. For our hackathon project, we selected quantum simulations as the focal point of our exploration. Given our collective backgrounds and our profound expertise in the domain, our team possesses a deep-seated interest in the intricate properties of physical systems. We anchored our investigation on the H_2 molecule, delving into its dynamic behavior in the presence of a magnetic field. For us, the choice of the Hydrogen *molecule* excitingly marks a notable departure from the textbook example of a Hydrogen atom, which as physics students we are all perhaps overly familiar with.

II Project Accomplishments

A Simulating the Ground State with VQE

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. We then transform this fermionic Hamiltonian into a qubit (spin) Hamiltonian suitable for quantum computation. For our simulation, we used the Jordan-Wigner Transformation, which provides a direct mapping of fermions to qubits.

Using the Variational Quantum Eigensolver(VQE), we determined the ground state of the H_2 molecule. We used the $TwoLocal$ ansatz in Qiskit, which alternates between R_y and C_Z gates.

B Simulating just the H_2 Hamiltonian

To determine the time evolution operator of the H_2 in the absence of an external magnetic field, we applied the Trotterisation method using Qiskit's $SuzukiTrotter$. When applied to an arbitrary state $|\psi\rangle$, we found that the evolution operator obtained from the first-order Trotterisation yields an expected energy that matches the exact energy. Moreover, the expected energy remains constant over the evolution because the Hamiltonian is not time-dependent, as seen in the below derivation:

$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$
$$= \sum_n e^{-iE_n t} C_n |n\rangle$$
$$\langle\psi(t)|H|\psi(t)\rangle = \sum_m e^{-iE_m t} e^{iE_n t} C_m^* C_n \langle m|H|n\rangle$$
$$= \sum_n E_n |C_n|^2$$

Also,

$$|\psi(0)\rangle = \sum_n C_n |n\rangle$$
$$\langle\psi(0)|H|\psi(0)\rangle = \sum_{mn} C_m^* C_n \langle m|H|n\rangle$$
$$= \sum_n E_n |C_n|^2$$

C Introducing a static perturbation with Trotterisation

Now we consider the time-evolution of the H_2 molecule when it is exposed to a weak static magnetic field in the $\hat{x}$ direction. The resultant Hamiltonian assumes the form

$$\hat{H}_{static} = \hat{H}_{H_2} + \epsilon H_{static}. \tag{1}$$

As the Hamiltonian in this case is more complex than the previous, We observed that by increasing the order of Trotterisation, the accuracy of the energy evolution fit improves. Because $\hat{H}_{static}$ is still time-independent, the expected value remains constant following the explanation in the previou section.

D Introducing a time-dependent perturbation using Riemann-Sums and Trotterisation

We now introduce a changing external magnetic field perturbation, which makes our Hamiltonian time-dependent $H(t)$. In general, the evolution operator of a time-dependent Hamiltonian cannot be expressed as the matrix exponential $U(t) = e^{-i\hat{H}t}$ which is required for Trotterisation. In this case, we have to discretize our Hamiltonian over the interval $t \in [0, \tau]$ into N partitions. Within these small partitions, we assume the Hamiltonian is constant, enabling Trotterisation to be used.

$$\lim_{N \to \infty} \left(\prod_{k=1}^{N} e^{-iH\left(\frac{k\tau}{N}\right)\frac{\tau}{N}} \right) |\psi(0)\rangle \approx |\psi(t)\rangle$$

We observe that the expected value of the energy of the above state at generally varies through time, which we expected as the Hamiltonian is time-dependent. By adding an exponential decay term to the time-dependent perturbations, we are ultimatey able to recover the ground state energy of the unperturbed case, further validating the correctness of our results.

E Taking things further: Demonstrating the Adiabatic Theorem

Having implemented trotterisation, we now have the machinery to accurately evolve time-dependent Hamiltonians. Let us now consider Hamiltonians of the special form

$$\hat{H}_{ad}(t) = \left(1 - \frac{t}{\tau}\right) \hat{H}_1 + \frac{t}{\tau} \hat{H}_2 \quad t \in [0, \tau]. \qquad (2)$$

As times elapses from $t = 0$ to $t = \tau$, this physically corresponds to a system in which we gradually switch off the Hamiltonian $\hat{H}_1$ and turn on $\hat{H}_2$. Markedly, in the limit of large τ, our system evolves *adiabiatically* under this Hamiltonian. This means that if we begin in the ground state of H_1 at $t = 0$, then evolving it under H_{ad}

to $t = \tau$ produces the ground state of H_2. This is known as the *Adiabatic Theorem* in quantum mechanics.

We will now demonstrate this for the case of a $\hat{z}$-aligned Hydrogen molecule initially exposed to a magnetic field in the $\hat{x}$ direction. As time evolves, the magnetic field in the $\hat{x}$ direction will be adiabatically turned off, and simultaneously, a new magnetic field in the $\hat{z}$ direction will be adiabatically introduced:

$$\hat{H}_{ad}(t) = \hat{H}_{H_2} + \left(1 - \frac{t}{\tau}\right) \hat{H}_x + \frac{t}{\tau} \hat{H}_z \quad t \in [0, \tau] \quad (3)$$

By the adiabatic principle, if we begin in the ground state of $\hat{H}_{H_2} + \hat{H}_x$ at $t = 0$, then we expect to end up in the ground state of $\hat{H}_{H_2} + \hat{H}_z$ at $t = \tau$

1. Strong Magnetic Field Limit

For scenarios where the magnitude of the magnetic field was substantial, the molecular energy of the H_2 turned out to be negligible when juxtaposed with the dominating magnetic field. The overarching energy landscape was primarily governed by the external magnetic field, rendering the intrinsic molecular structure to exert minimal influence on the total system energy. The result is a symmetry between the perturbations along the different axes, disregarding the orientation of the molecule.

2. Weak Magnetic Field Limit

Conversely, under weaker magnetic fields, the intrinsic energy and structure of the H_2 molecule began to play a pronounced role in the interaction. The molecule's inherent characteristics started to significantly influence the energy of the system as the overriding effect of the magnetic field lessened. The alignment of the molecule along the z-axis effects a greater impact from a magnetic field along the z-axis compared with a magnetic field in the xy-plane, so the ground state energy is lower in the presence of a perturbative magnetic field along the z-axis.