Hybrid Quantum-classical Strategies for Hydrogen Variational Quantum Eigensolver Optimization

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Abstract- ***This research focuses on enhancing the optimization process of the classical ground state energy for hydrogen molecules, which is known to be -1.1373 Ha. Various well-known optimization algorithms such as Gradient Descent Optimizer, Adagrad Optimizer, Adam Optimizer, RMSProp Optimizer, and Momentum Optimizer are employed to explore their convergence behavior and their proximity to the precise ground state energy. The analysis extends to examining potential energy curves to gain insights into the stability and reactivity of hydrogen molecules. A notable discovery is the outstanding performance of the Momentum Optimizer, which outperforms other algorithms by achieving a ground state energy of -1.13724 Ha after 40 steps. This consistent and exceptional performance establishes the Momentum Optimizer as the preferred choice. Additionally, a sensitivity analysis of parameters highlights the Momentum Optimizer's unique capability to avoid local minima, reinforcing its importance in optimizing quantum chemistry problems. Importantly, our sensitivity analysis consistently demonstrates the Momentum Optimizer's remarkable and reliable convergence to the exact ground state, irrespective of initial parameter settings. In summary, the study underscores the critical role of the Momentum Optimizer in navigating the complex energy landscapes specific to hydrogen molecules in quantum chemistry simulations.***

Indexed Terms- ***Ground State Energy, Hydrogen Molecules, Molecular Stability, Momentum Optimizer, Optimization Algorithms, Potential Energy Curves, Quantum Chemistry***

I. INTRODUCTION

In the rapidly evolving realm of information processing [1], quantum computing stands at the forefront, offering transformative capabilities that surpass the boundaries of classical computation. Unlike classical bits, quantum bits or qubits possess the ability to exist in multiple states simultaneously, enabling quantum computers to execute intricate calculations at unparalleled speeds. A primary objective of quantum computing is to devise methods and algorithms for computing molecular electronic ground and excited state energies [2] , along with their corresponding wave functions, from first principles. These eigenvalues and eigenvectors are derived from solving the time-independent electronic Schrödinger equation. Despite the emergence of sophisticated classical many-body techniques such as Density Matrix Renormalization Group (DMRG), selected configuration interaction (sCI), and coupled-cluster (CC) theory, accurately computing properties of quantum systems like ground-state energies remains challenging for large-scale systems due to computational complexity. However, with the rise of quantum algorithms like the Variational Quantum Eigensolver (VQE), the landscape offers promising alternatives that leverage quantum mechanics principles to transcend classical limitations. While traditional quantum algorithms like Quantum Phase Estimation (QPE) show theoretical prowess, their practical implementation on near-term Noisy Intermediate-Scale Quantum (NISQ) devices is hindered by the need for numerous qubits and gates. Similarly, the Full Configuration Interaction Quantum Eigensolver (FQE), while holding potential for precise quantum chemistry simulations, faces obstacles when deployed on NISQ devices due to inherent limitations. The intricate balance between the demand for accurate quantum computations and the constraints of current quantum hardware underscores the ongoing pursuit of

innovative quantum algorithms and hardware advancements to bridge the gap between theoretical potential and practical feasibility.

Amidst the array of quantum algorithms, the Variational Quantum Eigensolver (VQE) emerges as a leading contender for efficiently computing ground-state and excited-state energies of molecules. Noteworthy for its hybrid approach, VQE seamlessly integrates classical and quantum computation to overcome the limitations of current quantum hardware. Central to VQE is a variational parameterized ansatz—a flexible quantum circuit representation encapsulating a trial wave function. This key feature facilitates iterative parameter refinement, enabling VQE to navigate the intricate solution space and converge towards an approximation of the ground state. Subsequently, the ansatz parameters undergo iterative optimization on a classical computer using the Rayleigh-Ritz variational principle. This iterative process enhances energy computation precision, rendering VQE a versatile and efficient tool for quantum chemistry applications, harmonizing the theoretical capabilities of quantum algorithms with the practical constraints of modern quantum devices. To address challenges associated with optimizing hardware-efficient and chemically-inspired ansatz circuits, our approach involves employing various optimization techniques. We intend to explore and compare different quantum optimizers, including gradient descent, Adagrad, Adam, RMSProp, and Momentum optimizers. Leveraging a diverse set of optimization algorithms aims to pinpoint the most effective strategy for minimizing energy and obtaining accurate ground state results. Additionally, we plan to conduct a sensitivity analysis by varying the initial parameters of the ansatz circuits. This analysis will offer insights into the robustness [3] of our chosen ansatz circuits and shed light on how variations in initial parameters impact the optimization process

1.1 Description of The Variational Quantum Eigensolver (VQE)

The Variational Quantum Eigensolver (VQE) algorithm is a potent quantum computing technique devised to determine the ground-state energy of a specified quantum system [4]. It harnesses the variational principle, a fundamental tenet of quantum mechanics [5]. This principle dictates that for any trial wavefunction ψ, the expected value of the Hamiltonian (H) will invariably exceed or equal the minimum energy (E0), represented as:

$$E \geq \min_{\psi} \langle \psi | \widehat{H} | \psi \rangle \quad (1)$$

The aim of the VQE is to identify the parameterization of the quantum state in a manner that minimizes the expectation value of the Hamiltonian [6]. The molecular electronic Hamiltonian is expressed as follows:

$$H(x) = \sum_{pq} h_{pq}\, p^{\dagger} q \; + \sum_{pqrs} h_{pqrs}\, p^{\dagger} q^{\dagger} sr.$$

1.2 Hydrogen(H_2) Molecule

Hydrogen molecules, denoted as H_2, represent the simplest diatomic molecule composed of two hydrogen atoms. As a fundamental entity in chemistry and quantum physics, H_2 molecules play a crucial role in understanding molecular bonding and electronic structure. The hydrogen atoms in an H_2 molecule form a covalent bond , sharing electrons to achieve a stable, and lower energy state. This covalent bonding leads to the creation of molecular orbitals, and the study of H_2 serves as a cornerstone in exploring quantum mechanical principles in molecular systems. In our investigation, we aim to analyze the quantum aspects of the H_2 molecule, focusing on its ground state energy, optimization with various algorithms, sensitivity to initial parameters, and dissociation energy under different bond lengths.

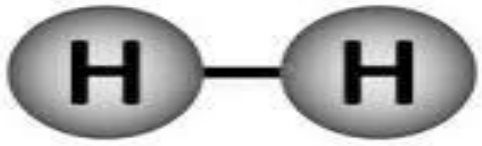

Figure 1. Hydrogen Molecules

In our implementation, we utilize the STO-3G basis set, which represents Slater Type Orbitals formed by a linear combination of 3 Gaussian functions. The convergence criterion was set to an order of 10^{-6} tolerance. In the next step, it is essential to establish the quantum circuit responsible for creating the trial

state of the molecule. Our objective is to generate states in the format.

$$|\psi(\theta)\rangle = cos\left(\frac{\theta}{2}\right)|1100\rangle - sin\left(\frac{\theta}{2}\right)|0011\rangle$$

In Jordan-Wigner encoding, the first term of the trial wave function $|\psi(\theta)\rangle$ represents the Hartree-Fock (HF) state. This encoding maps the HF state to a binary string, where each bit corresponds to the occupation of a specific molecular orbital. The second term encodes the double excitation, representing an electronic configuration where two electrons are excited from their initial orbitals to higher-energy orbitals and θ is the parameter to be optimized

II. RESULT AND DISCUSSION

In our investigation into quantum chemistry, we undertook a thorough study centered on simulating the stable energy state of H2 molecules. We utilized different optimization tools, including Gradient Descent Optimizer, Adagrad Optimizer, Adam Optimizer, and Momentum Optimizer. Our quantum system was described using a 4-qubit configuration and the STO-3G basis set. We rigorously examined the results, ensuring they met a strict convergence criterion of 10^{-6} tolerance. Additionally, our inquiry expanded beyond just the optimization outcomes to include a sensitivity analysis, where we closely observed how these optimization tools responded to variations in the conditions.

2.1 Analysis of optimizer performance

In this investigation, the classical ground state energy is established at -1.1373 Ha. The optimization results with Gradient Descent Optimizer, AdagradOptimizer, AdamOptimizer, RMSProp Optimizer, and Momentum Optimizer reveal convergent behaviors. Each optimizer demonstrates proximity to the exact ground state energy, with Momentum Optimizer showing the closest approximation, reaching -1.13700311 Ha after 40 steps. While all optimizers achieve close values, Momentum Optimizer stands out as the one converging most closely to the classical ground state energy, emphasizing its superior performance in this computational context.

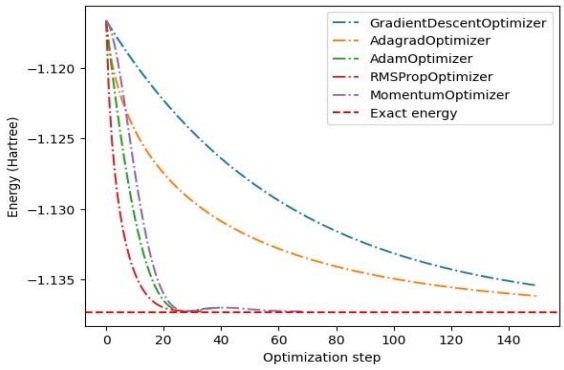

Figure 2. Convergence of Optimizers to Ground State Energy

2.2 Potential energy curve

The investigation focuses on potential energy, a critical parameter defining the stability and reactivity of molecular configurations [7]. The study entails the analysis of potential energy curves, offering essential insights into how the potential energy of a quantum system varies with different bond lengths. These curves serve as valuable tools for evaluating the stability of molecular configurations and comprehending the dynamics of chemical reactions. Remarkably, our research unveils a notable level of consistency among the results obtained using the four optimizers—Gradient Descent, Adagrad, Adam, and Momentum. These optimizers consistently converge to similar solutions for potential energy across diverse bond lengths, underscoring their resilience in navigating the potential energy landscape of quantum systems. However, the RMSProp Optimizer exhibits a distinct behavior. Initially, it diverges from the convergence observed with the other four optimizers but subsequently aligns with their solutions. This initial deviation and eventual convergence imply a unique exploration of the potential energy landscape by the RMSProp Optimizer, suggesting that it initially follows a different trajectory before converging to solutions akin to those obtained with the other optimizers.

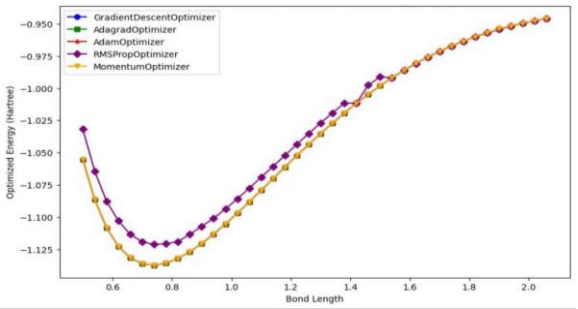

Figure 3 Potential energy curve for different optimizer

2.3 Parameter Sensitivity Analysis

Parameter sensitivity analysis is a critical component of optimizing quantum chemistry problems, as it sheds light on how different parameters and optimizers impact the optimization process. In our investigation, we explored the behavior of various optimizers across a range of initial parameter values to uncover intriguing trends. A standout finding from our sensitivity analysis was the consistently exceptional performance of the Momentum Optimizer. Irrespective of the initial parameter values, the Momentum Optimizer demonstrated a remarkable ability to converge to the exact ground state for the quantum computing problem. This robust convergence of the Momentum Optimizer is particularly noteworthy when compared to other optimizers in our study. While alternative optimizers struggled to locate the global minimum in certain scenarios, the Momentum Optimizer consistently reached the lowest energy state. Such remarkable performance underscores the Momentum Optimizer's effectiveness in escaping local minima and guiding the optimization process toward the global minimum. Our results underscore the significance of the Momentum Optimizer's capability to escape local minima for achieving precise and dependable outcomes in quantum chemistry simulations. In quantum systems, where accurately determining the ground state is paramount, the Momentum Optimizer's consistent and robust convergence establishes it as a valuable tool for optimizing quantum chemistry problems. In conclusion, the exceptional performance of the Momentum Optimizer in escaping local minima and achieving robust convergence underscores its importance in the domain of quantum chemistry optimization. As quantum simulations grow more complex, understanding optimizer nuances becomes essential for obtaining accurate and reliable results. The Momentum Optimizer emerges as a promising choice for such optimization tasks, demonstrating its efficacy in navigating the intricate energy landscapes of quantum systems.

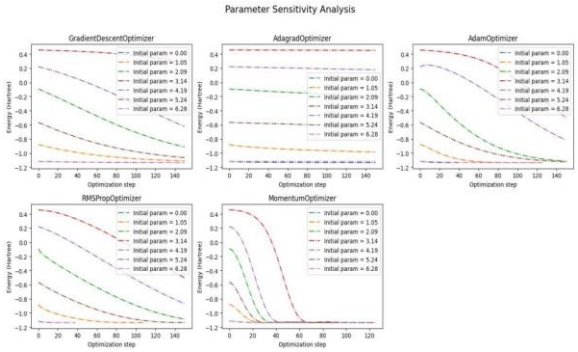

Figure 4. Parameter Sensitivity Analysis

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