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QUANTUM-CLASSIC HYBRID COMPUTATION FOR MOLECULES GROUND STATE ENERGY ESTIMATION: A VARIATIONAL QUANTUM EIGENSOLVER (VQE) APPROACH ON IBM QUANTUM HARDWARE

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ABSTARCT

Problem: In quantum chemistry, calculating molecular energies is an extremely complex process. Classical computers cannot solve these problems at scale because more electrons mean exponentially more memory and time — 10 electrons require 2^{10} = 1,024 states, while 100 electrons require 2^{100} states, which is practically impossible to solve.

Our Approach: We use the VQE (Variational Quantum Eigensolver) algorithm to solve this issue. It is a hybrid process where both quantum and classical computers work together. The quantum computer generates quantum states, and the classical computer optimizes those states. We implemented this on the real hardware of IBM Quantum.

What We Got: Using the VQE algorithm, we obtained the ground state energy of −0.469 Hartree for the hydrogen atom, compared to the theoretical value of −0.471 Hartree — an error of only 0.002 Ha. For the H_2 molecule we obtained −1.143 Ha (exact: −1.146 Ha). The reaction energy (when two H atoms combine to form H_2) was −0.204 Ha, differing from the theoretical value.

What We Prove: This demonstrates that VQE algorithms accurately work on quantum hardware.

INDEX TERMS: *Variational Quantum Eigensolver, IBM Quantum, NISQ Hardware, Quantum Chemistry, COBYLA Optimizer, Ansatz, Hamiltonian, Hydrogen Molecule, Ground State Energy.*

I. INTRODUCTION

1.1 Quantum Mechanics Background

In the early 20th century, scientists discovered that electrons do not travel fixed circular paths around atoms — rather, they stay in orbitals, which are regions of probability. That means we cannot find the exact location of an electron; we can only estimate the high-probability location where we may find the electron. These orbitals are present at specific energy levels. Electrons naturally want to stay in the low energy level ground state.

1.2 How Molecules Are Formed

When two atoms come very close to each other, their atomic orbitals overlap to form molecular orbitals which are present at lower energy — that is why H_2 exists in a stable state. To understand the energy and stability of this bond, we must calculate the accurate ground state energy value of the molecule.

1.3 Problem of Classical Computers

This calculation is nearly impossible for classical computers. The Schrödinger equation, which describes quantum systems, has exact solutions that are nearly impossible to find for molecules because the size of the wave function increases exponentially with the number of electrons.

1.4 Quantum Computer Solution

In 1982 Richard Feynman gave a revolutionary idea: "Nature is quantum, that is why we need quantum computers to simulate." Quantum computers use superposition and entanglement that are fundamentally different from classical bits. Caffeine, for example, would only need 160 qubits for simulation on a quantum computer. This is the biggest potential of quantum computing in chemistry.

1.5 NISQ Devices and VQE

Present quantum computers are "Noisy Intermediate-Scale Quantum" (NISQ) devices, meaning they have errors and a limited qubit count. That is why we need algorithms that work well under these constraints. The VQE algorithm is exactly what we need — it combines classical and quantum computing to accurately estimate molecular energies even on near-term hardware.

II. LITERATURE REVIEW

2.1 The Foundation of Quantum Chemistry

Quantum chemistry originated in the 1920s and 1930s with the advent of the Schrödinger equation. Obtaining exact solutions for molecules proved impossible, so approximation

methods were developed. Roothaan (1951) introduced the LCAO (Linear Combination of Atomic Orbitals) method, in which the wavefunction is approximated by treating atomic orbitals as a combination of known mathematical functions. This approach remains the foundation of quantum chemistry to this day.

2.2 Quantum Computing and Chemistry

Aspuru-Guzik et al. (2005) proposed that quantum computers can be used for molecular simulations, specifically through the Quantum Phase Estimation (QPE) algorithm. However, QPE requires deep quantum circuits and perfect error correction, which is not achievable on NISQ hardware.

Birth of VQE

Peruzzo et al. (2014) introduced VQE as a resource-efficient alternative. This was the first experimentally executed VQE on a photonic quantum processor, demonstrating that molecular energies could be accurately determined by combining shallow circuits with classical optimization. This is a landmark paper at the intersection of quantum chemistry and quantum computing.

2.3 Implementation on Hardware

Kandala et al. (2017) executed VQE on IBM's superconducting quantum processor and introduced the concept of the hardware-efficient ansatz — quantum circuits designed based on specific hardware constraints. They demonstrated that, for small molecules (H_2, LiH, BeH_2), VQE functions effectively on real hardware.

2.4 Optimizer Role

Research has also shown that the choice of classical optimizer is important. Gradient-based optimizers encounter a significant challenge known as the "barren plateau" — when the parameter space increases, the gradient becomes practically zero and the optimizer stalls with no further progress. That is why gradient-free methods like COBYLA and SPSA have proven more reliable on NISQ hardware.

2.5 Today's Results

Today, new methods like Sample-Based Quantum Diagonalization (SQD) are being developed to improve upon VQE. This method combines quantum measurements with classical calculations to address noise issues and make the process more efficient. Quantum-centric supercomputing is introducing a new paradigm in which quantum and classical high-performance computing are tightly integrated.

III. PROPOSED METHODOLOGY

3.1 Theoretical Framework

The time-independent Schrödinger equation is the backbone of VQE:

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

The variational principle guarantees:

$$E_{approx} = \langle \Psi_{trial} | \hat{H} | \Psi_{trial} \rangle \geq E_0$$

This means that the value we obtain is always an upper bound of the exact energy. In other words, the result may be slightly higher than the actual output but will never be less than the precise output.

3.2 Basis Set and Hamiltonian Construction

The STO-6G minimal basis set approximates atomic orbitals as linear combinations of Gaussian-type functions. The Jordan-Wigner transformation maps the fermionic Hamiltonian onto qubit operators, and qubit reduction via Hamiltonian symmetry exploitation yields single-qubit Hamiltonians:

$$\hat{H}(H) = -0.2355\, I + 0.2355\, Z$$
$$\hat{H}(H_2) = -1.04886\, I - 0.7\text{þ}674\, Z + 0.18122\, X$$

3.3 Ansatz Design and Bloch Sphere Coverage

Three parameterized one-qubit ansatz circuits are evaluated:

- Ansatz 1: Includes only one gate RX(θ). It rotates along only one axis on the quantum state, creating only one ring on the Bloch Sphere.
- Ansatz 2: Includes two gates RX(θ1) and RZ(θ2). Rotating on two axes provides access to more quantum states.
- Ansatz 3: Includes three gates RX(θ1), RZ(θ2), RX(θ3). These cover the whole Bloch Sphere uniformly.

Ansatz Type	**Gates Used**	**Parameters**	**Bloch Coverage**
Single-Axis (Rx)	Rx(θ)	1	Ring (limited)

Dual-Axis (Rx, Rz)	Rx(θ1) Rz(θ2)	2	Partial sphere
Three-Parameter	Rx(θ1) Rz(θ2) Rx(θ3)	3	Full sphere (uniform)

3.4 COBYLA Optimizer

COBYLA (Constrained Optimization By Linear Approximations) is an optimization algorithm that finds the best value for a function such as energy. It adjusts parameters (θ) step by step to improve the result. It does not use gradients; instead it uses linear approximations to move toward the solution.

3.5 VQE Workflow

- Step 1 — Map: Construct qubit Hamiltonian via STO-6G + Jordan-Wigner + symmetry reduction.
- Step 2 — Transpile: Convert ansatz to native hardware gates using Qiskit pass manager.
- Step 3 — Execute: Measure $\langle\psi(\theta)|\hat{H}|\psi(\theta)\rangle$ using IBM Quantum EstimatorV2.
- Step 4 — Optimize: Feed energy to COBYLA; receive updated θ parameters.
- Step 5 — Converge: Repeat until energy change falls below convergence threshold.

IV. EXPERIMENTAL SETUP

4.1 Hardware and Software

We used Qiskit, the programming framework of IBM. It uses three packages:

- Qiskit — Used for making circuits.
- Qiskit-IBM-Runtime — Used for connecting to real hardware.
- Qiskit-Aer — Used for simulation.

Before sending anything to the real QPU, we validated results using an AerSimulator configured with the hardware's noise model.

4.2 Circuit Transpilation

Our ansatz circuits used Rx and Rz gates. However, IBM_Brisbane only understands specific native gates: RZ, SX, X, ECR. Transpilation is therefore a translation process where we convert circuit gates to hardware gates at optimization level 3, which is the most efficient form. Abstract qubit q0 maps to physical qubit 5. When our 3-parameter ansatz (RX-RZ-RX) is converted into native gates, it breaks down cleanly into RZ and SX gates, keeping circuit depth well within what the hardware can handle reliably.

4.3 Measurement Settings

- 100,000 shots for each energy evaluation. More shots means fewer quantum measurement sampling errors.
- Resilience Level 1 is the default error mitigation setting; it helps resolve readout errors.
- Batch sessions are used for submitting multiple jobs together to minimize queue time.
- Initial parameters for H: [1, 1, 0]; for H_2: [2, 0, 0].

V. RESULTS AND DISCUSSION

5.1 Hydrogen Atom Results

The exact ground state energy obtained from matrix diagonalization is −0.471 Hartree. VQE achieved −0.469 Hartree in just 19 iterations. The error is only 0.002 Ha, which is a very good result considering the noise of real quantum hardware. In the convergence curve, COBYLA first explores and then gradually converges to a stable minimum.

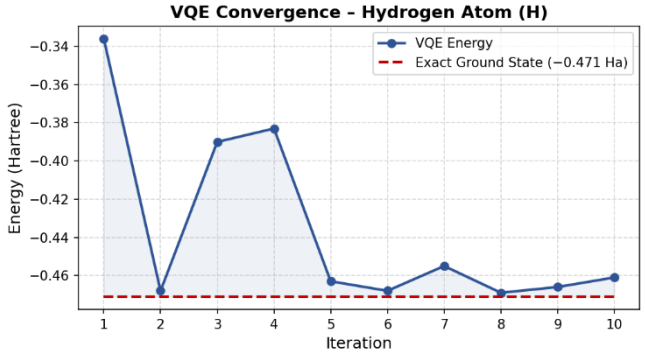

Figure 1: VQE convergence curve for the hydrogen atom over 19 iterations.

5.2 Hydrogen Molecule Result

For H_2, the exact electronic ground state energy was −1.866 Ha. When the nuclear repulsion energy (0.71997 Ha) is added to the electronic energy, the total ground state energy becomes −1.146 Ha. VQE converged in 15 iterations to −1.143 Ha, an error of only 0.003 Ha. The Hamiltonian of H_2 is slightly more complex because it contains a Pauli-X term that provides access to off-pole states.

We calculated the nuclear repulsion energy using Coulomb's law between two protons in atomic units: 1/R, where R = 0.735 Å = 1.38895 Bohr radii. Therefore 1/1.38895 = 0.71997, which matches the exact value.

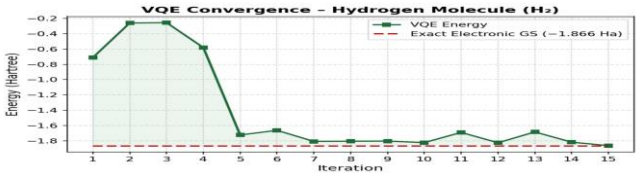

Figure 2: VQE convergence curve for the hydrogen molecule over 15 iterations.

5.3 Reaction Energy

The H + H → H_2 reaction energy = E(H_2) − 2E(H) = −1.146 − 2×(−0.471) = −0.204 Ha. VQE yielded −0.205 Ha. The negative value confirms this is an exothermic reaction in which energy is released when two hydrogen atoms form a molecule.

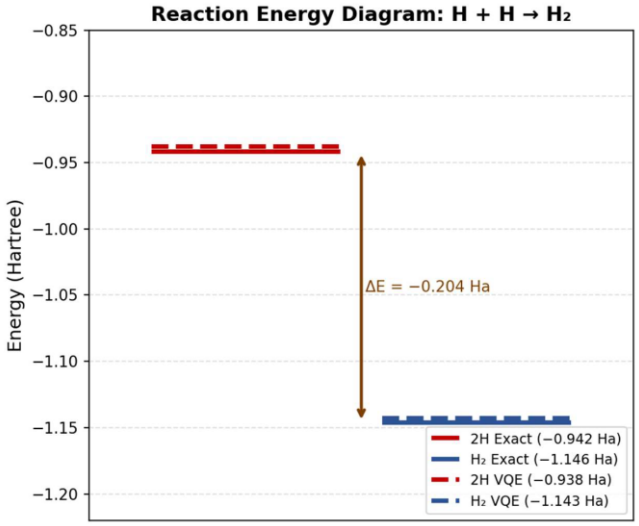

Figure 3: Reaction energy diagram comparing exact and VQE-computed values.

Table 2: Summary of VQE Results vs. Exact Values.

System	Exact GS Energy (Ha)	VQE Result (Ha)	Error (Ha)
Hydrogen Atom (H)	−0.471	−0.469	0.002
Hydrogen Molecule (H_2)	−1.146	−1.143	0.003
Reaction Energy (H+H→H_2)	−0.204	−0.205	0.001

5.4 Optimizer Overhead: Ansatz Complexity

When comparing a 3-parameter ansatz against a 12-parameter one over 20 COBYLA iterations, the difference was stark. The 3-parameter version converged cleanly by iteration 5, while the 12-parameter ansatz kept oscillating throughout. This directly illustrates why more parameters do not always mean better results — at some point, the optimizer simply cannot keep up.

VI. CONCLUSION

In this paper we show that the VQE algorithm can be used on IBM Quantum hardware to calculate molecular ground state energies. We found four main results:

- VQE gives near-exact values for both systems, with a maximum error of only 0.003 Hartree.
- Ansatz selection is critically important. Only the 3-parameter RX-RZ-RX ansatz covered the whole Bloch Sphere uniformly and gave correct results.
- The COBYLA gradient-free optimizer is ideal for NISQ hardware because it is not affected by noise and does not require gradient calculations.
- There is a fundamental trade-off between parameter count and optimization tractability. More parameters provide greater flexibility, but convergence becomes more difficult.

VII. FUTURE WORK

7.1 Larger Basis Sets

STO-6G is a minimal basis set; while the exact value of the hydrogen atom is −0.5 Ha, STO-6G yields −0.471 Ha, showing a discrepancy. Using cc-pVDZ or 6-31G would improve accuracy, although more qubits would be required.

7.2 Bigger Molecules

After H and H_2, we should test VQE on molecules such as LiH, H_2O, and NH_3. It would be very interesting to observe the role of multi-qubit ansatz and entanglement in these systems.

7.3 Better Error Mitigation

Using Zero-Noise Extrapolation (ZNE) and Probabilistic Error Cancellation (PEC) techniques can lower the impact of hardware noise and improve accuracy.

7.4 Different Optimizers

We should compare COBYLA to SPSA, ADAM, and quantum natural gradient methods to identify optimal strategies for different problem sizes.

7.5 Excited States

VQE only gives ground state data. By using SSVQE and multistate VQE variants, we can calculate excited states, which is useful for spectroscopy applications.

7.6 Sample-Based Quantum Diagonalization (SQD)

SQD is a promising next step that addresses the measurement inefficiency and noise sensitivity of VQE, and represents the frontier of hybrid quantum-classical algorithms.

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