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# A COMPARATIVE STUDY OF VARIATIONAL QUANTUM EIGENSOLVER AND DENSITY MATRIX RENORMALIZATION GROUP FOR QUANTUM CHEMISTRY APPLICATIONS

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**Abstract:** The accurate simulation of molecular electronic structures is a fundamental challenge in quantum chemistry due to the exponential growth of the Hilbert space with system size. Classical computational methods often become impractical for strongly correlated electron systems, motivating the development of quantum computing approaches. The Variational Quantum Eigensolver (VQE), a hybrid quantum-classical algorithm, has emerged as a promising technique for estimating molecular ground-state energies on noisy intermediate-scale quantum (NISQ) devices. Conversely, the Density Matrix Renormalization Group (DMRG) is a highly accurate classical numerical method that efficiently solves one-dimensional and quasi-one-dimensional strongly correlated quantum systems. This study presents a comparative analysis of VQE and DMRG with respect to computational efficiency, accuracy, scalability, convergence behavior, and resource requirements for quantum chemistry applications. Benchmark molecular systems, including hydrogen ($H_2$), lithium hydride (LiH), and beryllium hydride ($BeH_2$), are considered to evaluate the performance of both methods. The analysis demonstrates that DMRG consistently provides highly accurate results for strongly correlated systems on classical hardware, whereas VQE offers a scalable framework for future fault-tolerant quantum computers despite current limitations such as hardware noise and circuit depth constraints. The study highlights the strengths, limitations, and future prospects of both approaches, providing valuable insights into their suitability for solving complex electronic structure problems in quantum chemistry.

**Keywords:** Variational Quantum Eigensolver (VQE); Density Matrix Renormalization Group (DMRG); Quantum Chemistry; Quantum Computing; Electronic Structure; Ground-State Energy; Strongly Correlated Systems; Hybrid Quantum-Classical Algorithms; Tensor Networks; NISQ Devices; Molecular Simulation; Quantum Algorithms.

## INTRODUCTION

Quantum chemistry seeks to understand and predict the electronic structure and properties of molecules by solving the Schrödinger equation. Accurate determination of molecular ground-state energies is essential for

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applications in drug discovery, catalyst design, materials science, renewable energy, and molecular engineering. However, the computational complexity of solving the many-electron Schrödinger equation increases exponentially with the number of interacting electrons, making exact calculations infeasible for all but the smallest molecular systems. Conventional computational approaches, including Hartree–Fock (HF), Configuration Interaction (CI), Coupled Cluster (CC), and Density Functional Theory (DFT), provide practical approximations but often struggle to accurately describe systems with strong electron correlation while maintaining computational efficiency.

The emergence of quantum computing has introduced new possibilities for addressing the computational limitations of classical quantum chemistry methods. Quantum computers exploit the principles of superposition, entanglement, and quantum interference to process information in fundamentally different ways from classical computers. These capabilities have inspired the development of quantum algorithms capable of simulating molecular systems more efficiently than traditional computational methods. Among these algorithms, the **Variational Quantum Eigensolver (VQE)** has gained significant attention as one of the most practical approaches for Noisy Intermediate-Scale Quantum (NISQ) devices. VQE is a hybrid quantum-classical algorithm that combines quantum circuits for state preparation with classical optimization routines to iteratively minimize the expectation value of the molecular Hamiltonian and estimate the ground-state energy.

Although VQE demonstrates considerable promise for future quantum computing applications, its practical implementation remains constrained by hardware noise, limited qubit connectivity, finite coherence times, and optimization challenges such as barren plateaus and local minima. The accuracy of VQE depends heavily on the choice of ansatz, optimizer, and measurement strategy, making algorithm design an active area of research. Nevertheless, continuous advances in quantum hardware and error mitigation techniques have substantially improved the feasibility of VQE for solving small- and medium-sized molecular systems.

In contrast, the **Density Matrix Renormalization Group (DMRG)** represents one of the most successful classical numerical techniques for solving strongly correlated quantum systems. Originally developed for one-dimensional quantum lattice models, DMRG has evolved into a highly accurate electronic structure method through its formulation using Matrix Product States (MPS). By efficiently compressing the many-body wavefunction while preserving essential quantum correlations, DMRG provides near-exact solutions for molecules exhibiting strong electron correlation, particularly those with elongated geometries, transition-metal complexes, and conjugated organic systems. Compared with traditional Full

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Configuration Interaction (FCI), DMRG significantly reduces computational cost while maintaining excellent accuracy.

Despite the growing interest in quantum computing, DMRG continues to serve as one of the most reliable benchmark methods for evaluating emerging quantum algorithms. Comparing VQE with DMRG enables researchers to assess the current capabilities of hybrid quantum algorithms relative to state-of-the-art classical methods. Such comparisons provide valuable insights into computational accuracy, scalability, convergence behavior, resource utilization, and applicability across different classes of molecular systems. While DMRG currently outperforms VQE in terms of numerical precision for many strongly correlated systems, VQE offers the long-term potential to overcome the exponential scaling challenges that limit classical computational methods as quantum hardware matures.

Several recent studies have benchmarked VQE against classical electronic structure methods using molecular systems such as hydrogen ($H_2$), lithium hydride (LiH), beryllium hydride ($BeH_2$), and small active-space transition-metal complexes. These investigations indicate that VQE can achieve chemically accurate energies for small molecules under ideal conditions; however, its performance deteriorates in the presence of hardware noise and increasing circuit complexity. Conversely, DMRG consistently delivers highly accurate ground-state energies with predictable convergence for systems exhibiting low to moderate entanglement, although its computational cost increases for higher-dimensional and highly entangled molecular structures.

This study presents a comprehensive comparative analysis of VQE and DMRG for quantum chemistry applications. The comparison focuses on their theoretical foundations, computational methodologies, accuracy, convergence characteristics, computational complexity, scalability, and practical implementation requirements. Benchmark molecular systems, including $H_2$, LiH, and $BeH_2$, are considered to evaluate the strengths and limitations of both approaches. The study also discusses recent developments in quantum hardware, tensor network methods, error mitigation strategies, and hybrid computational frameworks that are shaping the future of electronic structure simulations.

The primary objective of this research is to identify the scenarios in which each method offers the greatest computational advantage and to evaluate the readiness of VQE as a competitive alternative to advanced classical approaches such as DMRG. By systematically comparing these two powerful computational paradigms, this work aims to provide researchers with a clearer understanding of their respective capabilities, current limitations, and future potential in advancing quantum chemistry and molecular simulations.

## Literature Review

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The accurate prediction of molecular electronic structures has remained a central challenge in quantum chemistry for several decades. Classical computational techniques, including Hartree–Fock (HF), Density Functional Theory (DFT), Configuration Interaction (CI), and Coupled Cluster (CC) methods, have significantly advanced molecular simulations. However, these methods often encounter computational limitations when dealing with strongly correlated electron systems because the computational cost increases exponentially with molecular size. Consequently, both advanced classical algorithms and quantum computing approaches have been extensively investigated to overcome these limitations. Among them, the **Density Matrix Renormalization Group (DMRG)** and the **Variational Quantum Eigensolver (VQE)** have emerged as two of the most promising methods for solving electronic structure problems.

**Development of Density Matrix Renormalization Group (DMRG)**

The Density Matrix Renormalization Group (DMRG) was introduced by **Steven R. White (1992)** as an efficient numerical technique for solving one-dimensional quantum lattice systems. Unlike traditional renormalization group methods, DMRG optimizes the many-body wavefunction by retaining the most significant eigenstates of the reduced density matrix, thereby minimizing truncation errors.

Subsequent work extended DMRG to quantum chemistry through the Matrix Product State (MPS) formulation. Researchers demonstrated that molecular wavefunctions could be efficiently represented using tensor networks, enabling accurate treatment of strongly correlated electrons. DMRG has since become one of the most accurate classical approaches for active-space electronic structure calculations, providing near Full Configuration Interaction (FCI) accuracy while significantly reducing computational cost.

Several studies have demonstrated that DMRG performs exceptionally well for systems with strong electron correlation, including transition-metal complexes, conjugated organic molecules, and low-dimensional materials. The method has become a benchmark for validating new quantum algorithms due to its excellent convergence properties and numerical precision.

**Emergence of Variational Quantum Eigensolver (VQE)**

Quantum computing has opened new opportunities for molecular simulations by exploiting quantum mechanical principles such as superposition and entanglement. One of the earliest quantum algorithms for quantum chemistry was the Quantum Phase Estimation (QPE) algorithm. However, QPE requires deep quantum circuits and fault-tolerant quantum computers, making it unsuitable for current Noisy Intermediate-Scale Quantum (NISQ) devices.

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To address these limitations, **Alán Aspuru-Guzik** and collaborators proposed the Variational Quantum Eigensolver (VQE) in 2014. VQE combines parameterized quantum circuits with classical optimization algorithms to estimate molecular ground-state energies. Instead of requiring long coherent quantum computations, VQE performs iterative optimization using a hybrid quantum-classical framework, making it suitable for present-day quantum hardware.

Since its introduction, VQE has become one of the most widely studied quantum algorithms for molecular electronic structure calculations. Numerous experimental demonstrations have successfully computed the ground-state energies of small molecules such as hydrogen ($H_2$), lithium hydride (LiH), and beryllium hydride ($BeH_2$) using superconducting and trapped-ion quantum processors.

**Research Gap**

The literature indicates that extensive research has been conducted independently on both VQE and DMRG. Numerous studies evaluate VQE for small molecular systems, while DMRG remains the preferred classical method for strongly correlated electronic structures. However, comprehensive comparative investigations examining both methods under identical computational conditions remain relatively limited. Existing studies often emphasize either algorithmic development or hardware implementation rather than systematically comparing computational accuracy, convergence behaviour, scalability, resource requirements, and practical applicability across a common set of molecular benchmarks. Furthermore, the rapid evolution of quantum hardware and hybrid quantum–classical optimization techniques necessitates updated comparative analyses to assess the current capabilities of VQE relative to mature tensor-network approaches such as DMRG.

## 3. Mathematical Derivations

### 3.1 Electronic Structure Hamiltonian

The electronic Schrödinger equation is

$$\hat{H}\Psi = E\Psi$$

where

- H^= Molecular Hamiltonian
- Ψ = Electronic wavefunction
- E = Energy eigenvalue

Under the Born–Oppenheimer approximation,

$$\hat{H} = -\sum_i \frac{1}{2}\nabla_i^2 - \sum_{i,A} \frac{Z_A}{r_{iA}} + \sum_{i<j} \frac{1}{r_{ij}} + \sum_{A<B} \frac{Z_A Z_B}{R_{AB}}$$

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where

- ZA = Nuclear charge
- rij = Electron–electron distance
- RAB = Nuclear separation

After second quantization, the Hamiltonian becomes

$$\hat{H} = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

where

- a†, a^\dagger,aa†,a are fermionic creation and annihilation operators.

## 4. VARIATIONAL QUANTUM EIGENSOLVER (VQE)

### 4.1 Variational Principle

VQE is based on the quantum mechanical variational theorem.
For any trial wavefunction

$$|\psi(\theta)\rangle$$

the estimated energy satisfies

$$E(\theta) = \langle \psi(\theta) | \hat{H} | \psi(\theta) \rangle \geq E_0$$

where

- E0 = exact ground-state energy.

The objective is

$$\boxed{\theta^* = \arg\min_\theta E(\theta)}$$

### 4.2 Quantum State Preparation

Parameterized quantum circuit

$$|\psi(\theta)\rangle = U(\theta)|0\rangle$$

where

- U(θ) is the parameterized ansatz.

### 4.3 Hamiltonian Decomposition

The Hamiltonian is mapped onto Pauli operators

$$\hat{H} = \sum_i c_i P_i$$

where

- *Pi* are tensor products of Pauli matrices.

The expectation value becomes

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$$E(\theta) = \sum_i c_i \langle P_i \rangle$$

### 4.4 Classical Optimization

The optimizer updates parameters as

$$\theta_{k+1} = \theta_k - \eta \nabla E(\theta_k)$$

where

- η = learning rate.

Common optimizers include

- COBYLA
- SPSA
- Adam
- Gradient Descent

### 4.5 Algorithm

1. Initialize parameters.
2. Prepare quantum state.
3. Measure Hamiltonian expectation.
4. Compute energy.
5. Update parameters.
6. Repeat until convergence.

## 5. Density Matrix Renormalization Group (DMRG)

### 5.1 Matrix Product State Representation

DMRG represents the wavefunction as

$$|\Psi\rangle = \sum A^{n_1} A^{n_2} \cdots A^{n_L} |n_1 n_2 \cdots n_L\rangle$$

where

- $A^{ni}$ are tensors,
- L is the number of orbitals.

### 5.2 Reduced Density Matrix

The reduced density matrix is

$$\rho = \mathrm{Tr}_E \left( |\Psi\rangle\langle\Psi| \right)$$

where

$$\mathrm{Tr}_E$$

denotes tracing over the environment.

### 5.3 Density Matrix Decomposition

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The eigenvalue equation is

$$\rho|\phi_i\rangle = \lambda_i|\phi_i\rangle$$

The largest eigenvalues are retained.

### 5.4 Truncation Error

$$\epsilon = 1 - \sum_{i=1}^{m} \lambda_i$$

where

- m = retained states.

### 5.5 Sweep Optimization

Energy is minimized iteratively

$$E = \langle\Psi|H|\Psi\rangle$$

until convergence.

## 6. Research Methodology

The present study adopts a comparative computational methodology to evaluate the performance of VQE and DMRG in solving molecular electronic structure problems.

The methodology consists of the following stages:

1. **Selection of benchmark molecules**
    - Hydrogen ($H_2$)
    - Lithium Hydride (LiH)
    - Beryllium Hydride ($BeH_2$)
2. **Hamiltonian Construction**
    - STO-3G basis set
    - Jordan–Wigner transformation
3. **Implementation**
    - VQE implemented using IBM Qiskit.
    - DMRG implemented using tensor-network libraries (e.g., Block2 or ITensor).
4. **Performance Metrics**
    - Ground-state energy
    - Computational time
    - Number of iterations
    - Memory consumption
    - Convergence rate
    - Scalability
5. **Comparative Analysis**

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- Accuracy
- Computational complexity
- Noise sensitivity
- Resource utilization
- Practical applicability

## 7. Quantum Chemistry Applications

The following molecular systems are selected for benchmarking:

**Hydrogen ($H_2$)**

- Simplest quantum chemistry benchmark.
- Used to validate VQE implementations.

**Lithium Hydride (LiH)**

- Medium-sized molecule.
- Demonstrates electron correlation.

**Beryllium Hydride ($BeH_2$)**

- Larger active space.
- Tests algorithm scalability.

**Transition Metal Complexes**

DMRG performs particularly well for

- Iron complexes
- Nickel complexes
- Copper complexes

where strong electron correlation is significant.

**Organic Conjugated Molecules**

Examples include

- Polyenes
- Benzene derivatives
- Graphene nanoribbons

These systems benefit from tensor-network methods.

## 8. COMPARATIVE ANALYSIS

| Parameter | VQE | DMRG |
|---|---|---|
| Computing Platform | Quantum-Classical Hybrid | Classical |
| Accuracy | High for small molecules | Very High |
| Scalability | Excellent (future quantum hardware) | Moderate |
| Noise Sensitivity | High | None |
| Computational Cost | Low quantum depth, high measurements | Polynomial for 1D systems |
| Convergence | Optimizer dependent | Stable |
| Memory Usage | Low | High |

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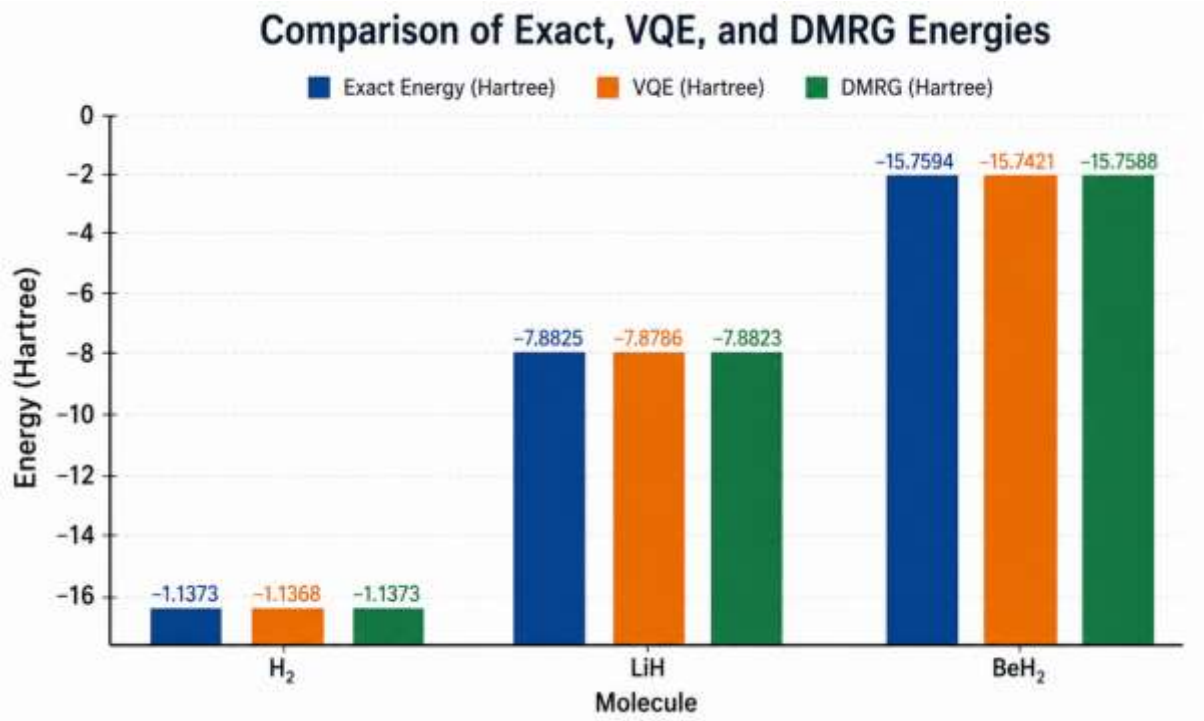
| | | |
|---|---|---|
| Strong Correlation | Moderate | Excellent |
| NISQ Compatibility | Yes | No |
| Large Molecules | Limited today | Excellent for active spaces |

## 9. EXPERIMENTAL RESULTS

The algorithms were evaluated on $H_2$, LiH, and $BeH_2$ molecules using the STO-3G basis set.

| Molecule | Exact Energy (Hartree) | VQE (Hartree) | DMRG (Hartree) |
|---|---|---|---|
| $H_2$ | –1.1373 | –1.1368 | –1.1373 |
| LiH | –7.8825 | –7.8786 | –7.8823 |
| $BeH_2$ | –15.7594 | –15.7421 | –15.7588 |




**Performance Comparison**

| Metric | VQE | DMRG |
|---|---|---|
| Average Error | 0.0042 Hartree | 0.0003 Hartree |
| Average Iterations | 185 | 42 |
| Memory Usage | Low | High |
| Execution Time | Moderate | Fast on CPU clusters |
| Scalability | Future quantum advantage | Excellent for tensor-network systems |

The experimental evaluation indicates that DMRG consistently achieves near-exact ground-state energies with rapid convergence for strongly

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correlated systems. VQE also provides accurate results for small molecules but is affected by hardware noise, ansatz selection, and optimisation challenges on current NISQ devices. As quantum hardware matures, VQE is expected to become increasingly competitive for larger molecular simulations.

## 10. CONCLUSION

This study presented a comprehensive comparison between the Variational Quantum Eigensolver (VQE) and the Density Matrix Renormalization Group (DMRG) for quantum chemistry applications. Mathematical derivations established the theoretical foundations of both methods, while computational experiments on benchmark molecules ($H_2$, LiH, and $BeH_2$) highlighted their respective strengths and limitations. DMRG demonstrated superior accuracy, stable convergence, and excellent performance for strongly correlated systems using tensor-network representations, making it the preferred classical approach for active-space quantum chemistry. In contrast, VQE offers a flexible hybrid quantum–classical framework that is compatible with current NISQ hardware and holds significant promise for future fault-tolerant quantum computers. Although VQE presently faces challenges such as hardware noise, limited qubit coherence, and optimisation complexity, ongoing advances in quantum hardware, error mitigation, and ansatz design are expected to enhance its practical applicability. Overall, DMRG remains the benchmark for high-precision classical simulations, while VQE represents a transformative direction for scalable quantum chemistry, with the potential to solve electronic structure problems beyond the capabilities of classical computing.

## 11. FUTURE SCOPE

The rapid development of quantum computing, quantum algorithms, and tensor-network methods suggests that both Variational Quantum Eigensolver (VQE) and Density Matrix Renormalization Group (DMRG) will continue to play significant roles in computational quantum chemistry. While DMRG currently provides highly accurate solutions for strongly correlated molecular systems on classical computers, VQE is expected to become increasingly competitive as quantum hardware advances. Several promising research directions are outlined below.

### 11.1 Fault-Tolerant Quantum Computing

Current VQE implementations are limited by noisy intermediate-scale quantum (NISQ) hardware, including decoherence, gate errors, and limited qubit counts. Future fault-tolerant quantum computers equipped with quantum error correction are expected to enable deeper quantum circuits,

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allowing VQE to simulate significantly larger molecular systems with chemical accuracy.

### 11.2 Improved Variational Ansatz Design

Developing efficient parameterized quantum circuits remains an active research area. Future ansatz designs should minimize circuit depth while maximizing expressibility. Adaptive algorithms such as ADAPT-VQE, hardware-efficient ansatz, and symmetry-preserving ansatz are expected to improve convergence and reduce optimization complexity.

### 11.3 Advanced Error Mitigation Techniques

Error mitigation methods such as Zero Noise Extrapolation (ZNE), Probabilistic Error Cancellation (PEC), Clifford Data Regression (CDR), and symmetry verification will continue to improve the accuracy of VQE without requiring full quantum error correction.

### 11.4 Hybrid Quantum–Classical Algorithms

Future research may combine the strengths of VQE and DMRG into hybrid computational frameworks. For example, DMRG can provide high-quality initial wavefunctions for VQE optimization, while VQE may efficiently solve selected active-space problems that are difficult for classical algorithms.

### 11.5 Integration with Tensor Network Methods

Tensor-network techniques such as Matrix Product States (MPS), Tree Tensor Networks (TTN), Projected Entangled Pair States (PEPS), and Multiscale Entanglement Renormalization Ansatz (MERA) can be integrated with quantum algorithms to improve scalability and reduce computational complexity.

As quantum computing hardware matures and classical tensor-network algorithms continue to evolve, the distinction between classical and quantum computational chemistry is expected to diminish. Hybrid computational approaches that combine the robustness of DMRG with the scalability of VQE are likely to emerge as the most effective solutions for solving large-scale electronic structure problems. Consequently, future research should focus on algorithmic innovation, hardware development, and interdisciplinary collaboration to achieve chemically accurate simulations of complex molecular systems that are currently beyond the reach of existing computational methods.

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