QUANTUM COMPUTING FOR PHYSICAL SYSTEM MODELLING AND SIMULATION: A COMPREHENSIVE REVIEW

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ABSTRACT

Quantum computing has become a revolutionary paradigm, providing solutions to complex computational problems that are impossible for traditional classical systems. One of its most promising uses is in modeling and simulating physical phenomena, which advances fields such as physics, chemistry, materials science, and engineering. This article offers an in-depth review of recent breakthroughs in quantum computing related to modeling and simulating physical systems. We examine the core principles of quantum algorithms, including variational quantum eigenvalue solvers (VQEs), quantum approximate optimization algorithms (QAOAs), and quantum phase estimation (QPEs), focusing on their applications to simulating molecular structures, condensed matter systems, and dynamical processes. The review also discusses improvements in quantum hardware, error correction techniques, and hybrid quantum-classical methods that have increased the simulation capabilities of current noisy intermediate-scale quantum (NISQ) devices. Moreover, it explores challenges such as scalability, decoherence, and algorithmic efficiency, along with emerging solutions to enable practical use. By reviewing the latest research, this overview highlights future directions in quantum computing, which could greatly enhance the accuracy, speed, and range of modeling complex physical systems, bridging the gap between theory and realworld application.

KEYWORDS

Quantum Computing, Quantum Simulation, VQE, NISQ.

1. INTRODUCTION

Quantum computing is at the forefront of technological innovation and promises to fundamentally change how we solve complex problems across science and industry. By harnessing quantum mechanical principles such as superposition, entanglement, and quantum parallelism, quantum computers are expected to deliver exponential improvements over traditional systems, especially when dealing with large datasets or intricate physical phenomena. This research paper explores three main areas of quantum computing: quantum machine learning techniques, the application of neural networks to quantum many-body systems, and quantum simulation of physical phenomena. Quantum machine learning methods, including quantum support vector machines, quantum neural networks, quantum decision trees, and the Haro-Hasidim-Lloyd algorithm, aim to enhance conventional machine learning tasks like classification and optimization although they face challenges related to hardware noise and theoretical limits. Meanwhile, neural networks, particularly restricted Boltzmann machines, have advanced the study of quantum many-body systems by effectively modeling complex quantum states in models such as the transverse field Ising model and the Heisenberg model [1]. Their innovative

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architectures and training approaches have broadened theoretical understanding. Quantum simulation, a key aspect of quantum computing, allows detailed characterization of physical systems from molecular structures in quantum chemistry and correlated materials in condensed matter physics to lattice gauge theories in high-energy physics providing insights beyond the capabilities of classical methods. Despite significant potential, many challenges remain, including the limited number of qubits, noise in noisy intermediate-scale quantum (NISQ) devices, and issues related to algorithm scalability [2]. This article examines these interconnected topics, highlighting recent advances, ongoing obstacles, and future prospects. By integrating quantum computing into practical applications, this work emphasizes the transformative potential of these technologies to revolutionize research in artificial intelligence, materials science, and fundamental physics. The main contribution of this paper are as follows:

- This article argues that quantum computing is transforming our ability to simulate physical systems, offering a comprehensive synthesis of advancements across physics, chemistry, engineering, and materials science.
- We critically examine quantum algorithms including Variational Quantum Eigensolvers (VQEs), Quantum Approximate Optimization Algorithms (QAOAs), and Quantum Phase Estimation (QPE) evaluating their suitability, benefits, limitations, and effectiveness when implemented on noisy, medium scale quantum devices.
- This review also covers recent developments in quantum hardware, error correction techniques, and hybrid quantum-classical methodologies, emphasizing how these innovations can support practical applications in industry, research, and technology despite the current limitations and constraints of quantum platforms.
- Furthermore, we identify key challenges, including issues of scalability, decoherence, and algorithmic efficiency, and propose future research directions that can lead to hardware improvements, interdisciplinary applications, and innovative algorithm development all with the aim of enhancing the real-world practicality and impact of quantum simulation.

2. RELATED WORK

The concept of quantum simulation originates from Feynman's groundbreaking idea that the most effective way to model a quantum system is using the quantum components themselves. This claim laid the groundwork for quantum computing to become a powerful tool in physics and chemistry [1]. Lloyd later formalized the idea of a universal quantum simulator, showing that any local quantum system can be effectively replicated with quantum gates [2]. These fundamental studies led to the development of algorithms, especially quantum phase estimation (QPE) and its use in eigenvalue problems [3], and the Haro-Hasidim-Lloyd (HHL) algorithm for solving linear systems. The emergence of noisy intermediate-scale quantum (NISQ) devices has shifted focus toward hybrid techniques. Key approaches, like the variational quantum eigenvalue solver (VQE) [4] and the quantum approximate optimization algorithm (QAOA) [5], combine quantum state preparation with classical optimization. Further theoretical progress has deepened understanding of these algorithms, tackling issues such as expressiveness, optimization landscapes, and scalability. In quantum chemistry, [6] pioneered quantum algorithms for calculating molecular energies, while [7] carried out variational quantum eigenvalue calculations on superconducting qubits [8] extended these methods with photonic hardware, demonstrating the feasibility of small-scale chemical simulations. Later advances introduced efficient mappings like the transform [9] and resource reduction strategies [10] to lower the computational cost of electronic structure calculations. Progress has also been made in Hamiltonian simulation techniques. Trotter-Suzuki decomposition [11], deep chemical circuit implementations [12], and qubitization methods [13] achieve near-optimal resource scaling for simulating time evolution. Kassal et al. [14] demonstrated a polynomial-time quantum algorithm for chemical dynamics, bridging quantum information science and computational chemistry. With ongoing development of quantum hardware, error mitigation and correction strategies are increasingly important. Temme

et al. [15] proposed techniques like zero-noise extrapolation and probabilistic error elimination for shallow circuits. Babbush and colleagues [16] enhanced circuit design, resource estimation, and error-aware methods to enable practical nearterm simulations. On the software side, [17] has become a key framework, linking quantum chemistry models with efficient quantum circuit synthesis. Recent research also emphasizes interdisciplinary and hybrid methods. Tensor networks [18] offer efficient hybrid quantum-classical representations for many-body systems, while hybrid digital-analog schemes and retrieval-enhanced learning expand capabilities of near-term devices. Collectively, these advances mark the evolution of quantum simulation from theoretical concepts to experimental implementations and scalable computational frameworks.

Table 1 summarizes key contributions and challenges in the evolution of quantum simulation research, highlighting both foundational theories and practical limitations. Feynman first proposed quantum computers as natural simulators for physical systems, though no practical algorithms or hardware existed. Lloyd advanced this vision by formalizing universal quantum simulators with quantum gates, but these remained theoretical without implementation. Abrams and Lloyd introduced quantum phase estimation (QPE) for eigenvalue problems, yet the requirement for fault-tolerant quantum hardware made it unsuitable for noisy intermediate-scale quantum (NISQ) devices. Aspuru-Guzik et al. and Kassal et al. demonstrated quantum algorithms for molecular energies and chemical dynamics, but both required more qubits and gates than available. Harrow et al. (HHL) proposed a linear systems algorithm with exponential speedup, dependent on quantum RAM, while Lanyon et al. achieved experimental quantum chemistry simulations, limited to very small molecules. Seeley et al. introduced Bravyi– Kitaev encoding to reduce overhead, and Peruzzo et al. proposed the Variational Quantum Eigensolver (VQE), though both remained constrained by qubit demands and noise. Farhi et al. introduced QAOA, while McClean et al. analyzedvariational methods, uncovering barren plateau issues. O'Malley et al. experimentally implemented VQE on superconducting qubits for H_2, proving feasibility at small scales. Efforts to address hardware issues included Temme et al.'s error mitigation, Bravyi et al.'s qubit tapering, and Kivlichan et al.'s linear-depth circuits, though coherence and fidelity challenges persisted. Low and Chuang achieved theoretical optimal scaling via qubitization, still beyond NISQ limits. More recent works by Zhang & Tao and Bi link quantum simulation with AI and IoT, while Rani & Jain explore sentiment-based hybridization with NLP, and Danyal et al. assess classical NB approaches for simulation datasets. Collectively, these works show a clear trajectory from theory to smallscale demonstration, with progress constrained by current hardware limitations.

Table 1: Overview of Prior Research on Quantum Computing for Modeling and Simulating Physical Systems

Contributions	Key Issues
Proposed quantum computers as natural simulators for physical systems.	No practical algorithms or hardware existed to realize the idea.
Formalized universal quantum simulators using quantum gates.	Theoretical only; lacked concrete implementations and hardware validation.
Introduced QPE for eigenvalue problems.	Required fault-tolerant quantum hardware; not feasible on NISQ devices.
Demonstrated quantum algorithms for molecular energy calculations.	Resource requirements too large for existing quantum devices.
Polynomial-time quantum algorithm for chemical dynamics.	Practical implementation hindered by qubit and gate limitations.
Proposed linear systems algorithm with exponential speedup.	Dependent on quantum RAM and error-free operations; impractical on NISQ hardware.
Experimental quantum chemistry simulation using photonics.	Small-scale molecules only; scaling remained unresolved.
Introduced Bravyi–Kitaev mapping for fermion-to-qubit encoding.	Reduced overhead but still required many qubits for real molecules.
Introduced Variational Quantum Eigensolver (VQE) for chemistry.	Sensitive to noise and optimization challenges; limited scalability.
Proposed Quantum Approximate Optimization Algorithm (QAOA).	Algorithm depth and performance not well understood for large systems.
Analyzedvariational algorithms (VQE, QAOA).	Showed barren plateaus problem in optimization; scalability issues persisted.
Experimental VQE on superconducting qubits for H_2.	Demonstration limited to very small molecules.
Developed error mitigation for shallow circuits.	Does not eliminate noise; overhead still significant.
Introduced qubit tapering to reduce simulation overhead.	Gains limited to specific Hamiltonians with symmetries.
Optimized linear-depth circuits for electronic structure.	Still constrained by coherence times and gate fidelities.
Proposed qubitization and quantum signal processing.	Optimal scaling achieved theoretically; yet beyond NISQ capability.
Surveyed Artificial Intelligence of Things (AIoT) including quantum simulation links.	Focused more on AI integration; quantum hardware aspects unexplored.
Survey on AI-aided IoT, connecting to physical modeling.	Did not provide detailed algorithmic pathways for quantum simulation.
Aspect-based sentiment (cross-field, hybrid with NLP).	Illustrates trend toward hybridization; less emphasis on physics modeling.
Comparative NB approaches for simulation-related data sets.	Classical-leaning; gap remains in bridging scalable quantum simulation.

3. MATERIAL AND METHODS

This review employed a systematic methodology involving the collection, selection, classification, and analysis of scholarly works to highlight recent advancements in quantum computing for modeling and simulating physical systems. Relevant publications were gathered from various sources, using keywords including quantum computing, quantum simulation, physical modeling, VQE, QPE, QAOA, hybrid quantum-classical approaches, and NISQ devices. The scope of this review spanned publications from 1982 to 2024, covering foundational theories, algorithm development, experimental studies, and hardware innovations. To be included, studies needed to present theoretical frameworks, practical implementations, or address key challenges like scalability, decoherence, and error mitigation. Studies that were irrelevant or overly speculative were excluded. The selected literature was organized into five main categories: fundamental theory, core algorithms, applications in quantum chemistry and physics, resource optimization and error correction techniques, and advancements during the NISQ era. We then analyzed these works to identify their primary contributions, limitations, and emerging trends,

crossverifying findings across multiple studies to ensure reliability. This comprehensive approach offers a clear overview of the field's progression, emphasizing significant achievements, persistent challenges, and new opportunities for quantum simulations of physical systems. The development of this review adhered to a systematic methodology to guarantee thorough coverage and a critical assessment of existing research on quantum computing for the modeling and simulation of physical systems.

3.1 Analytical Approach

A comparative examination of the classified literature was performed to discern emerging research trends, strengths, weaknesses, and unresolved issues. The primary areas of focus included:

- The scalability of algorithms and their compatibility with hardware constraints.
- The balance between precision and resource consumption.
- The progression from theoretical concepts to experimental validations. Existing practical limitations in current NISQ device implementations.
- Potential future avenues, such as fault-tolerance techniques, hybrid quantum-classical models, and integration with traditional high-performance computing frameworks.

Figure 1 depicts a structured research framework comprising five sequential stages: literature collection, selection, classification, analysis, and synthesis of conclusions and future research directions. The process begins with literature collection, which serves as the foundation for any scholarly inquiry. In this phase, researchers gather extensive sources, including journal articles, conference papers, books, technical reports, and online repositories, to capture current knowledge and ongoing advancements in the selected field. Following collection, the next step is selection, where researchers critically assess and filter the gathered materials, retaining only those that are most relevant, credible, and aligned with the research objectives. This ensures a focused and trustworthy foundation for the study. The subsequent stage, classification, involves organizing the chosen literature into meaningful categories or themes, such as methodologies, algorithms, application domains, or challenges. This step provides structure to the research and facilitates the identification of commonalities, differences, and emerging trends across studies. After classification, the analysis phase commences, during which researchers conduct a thorough evaluation of the organized literature. This includes identifying strengths and limitations, uncovering research gaps, making comparisons, and synthesizing insights to deepen understanding of the topic. The final stage, conclusions and future directions, summarizes the overall findings, clearly outlining the current state of research. This phase also emphasizes the contributions of the reviewed work while pinpointing unresolved issues, unanswered questions, and potential avenues for future investigation. Overall, this systematic approach not only ensures a comprehensive and critical review of existing literature but also provides a solid foundation for new contributions, positioning the research within the wider scholarly discourse.

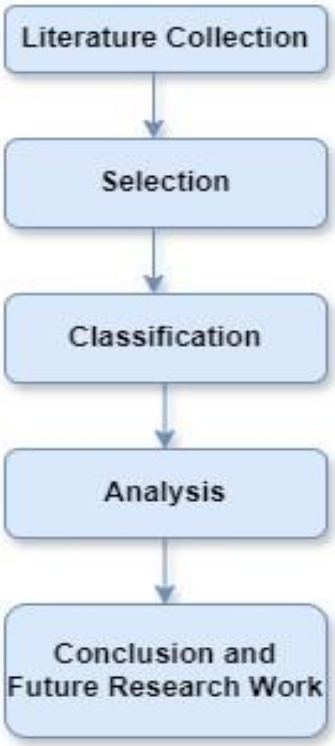

Figure 1: Flow the Step of Research Work

4. KEY CHALLENGES METHODS AND APPLICATIONS

4.1 Key Challenges

Quantum computing for modeling physical systems currently faces various technical and theoretical hurdles that limit its potential. Scalability remains a significant challenge, as noisy intermediate-scale quantum (NISQ) devices offer a limited number of qubits and short coherence durations, restricting the ability to perform large-scale simulations. Furthermore, noise and decoherence further impair performance, as quantum circuits are highly susceptible to environmental perturbations and imperfect gate operations. Many algorithms also face significant complexity, often requiring deep quantum circuits or complex optimizations that are impractical for existing hardware. While various error mitigation strategies have been devised, achieving comprehensive fault-tolerant quantum error correction remains resource-intensive and beyond current technological capabilities. Hardware limitations, such as limited connectivity, gate fidelity issues, and differences in qubit quality across different platforms (e.g., superconducting, trapped ion, and photonic systems), further hinder widespread adoption [19]. Finally, inherent optimization challenges in variational methods (such as VQE and QAOA), particularly the barren plateau problem, complicate efficient parameter training and reduce their practical application in real-world simulations.

4.2 Methods

To overcome these challenges, researchers have devised a variety of strategies to improve the efficiency and practicality of quantum computing in modeling physical systems. Variational algorithms (such as VQE and QAOA) and other hybrid quantum-classical solvers help minimize circuit depth, making them more compatible with NISQ devices. Hamiltonian simulation

techniques, including Trotter-Suzuki decomposition, qubitization, and quantum signal processing, improve the accuracy of time-evolution modeling. Efficient encoding and mapping methods, such as the Jordan-Wigner transform and the Bravyi-Kitaev transform, facilitate accurate representation of fermionic systems on quantum hardware. Furthermore, error mitigation techniques, such as zeronoise extrapolation, probabilistic error elimination, and symmetry verification, offer methods for reducing the effects of noise without requiring full fault tolerance [20]. Hybrid frameworks combining classical optimizers with quantum subroutines have demonstrated success in extending computational capabilities within current hardware limitations. Finally, resource optimization strategies, including circuit compression, qubit tapering, and symmetry exploitation, help reduce overall hardware requirements, thereby improving scalability and performance.

4.3 Applications

Quantum computing techniques for modeling physical systems have found applications across a broad spectrum of scientific and industrial fields. In quantum chemistry, they are employed to determine molecular ground-state energies, electronic configurations, and reaction mechanisms. In condensed matter physics, these methods facilitate the simulation of spin networks, phase transitions, and highly correlated materials. Materials science has also benefited through electronic structure predictions that aid in designing innovative catalysts, superconductors, and nanostructures. In high-energy physics, quantum approaches are used to investigate lattice gauge theories, particle interactions, and various aspects of quantum field simulations. Beyond fundamental research, optimization challenges in industries related to physics have been tackled using algorithms like the Quantum Approximate Optimization Algorithm (QAOA), addressing tasks such as logistics, scheduling, and resource management. Additionally, interdisciplinary applications are emerging, where tensor networks, artificial intelligence techniques, and hybrid high-performance computing (HPC) quantum frameworks are integrated to enhance scalability and expand the capabilities of quantum simulations.

5. Conclusion And Future Research Directions

Quantum computing promises to revolutionize how we model and simulate physical systems. Recent advances in quantum hardware and algorithms have demonstrated the ability to simulate complex quantum phenomena that are beyond the reach of conventional computers. Fields such as materials science, quantum chemistry, and condensed matter physics stand to benefit significantly, particularly through hybrid quantum-classical approaches that can improve the accuracy and effectiveness of simulations. For example, Google's development of a hybrid quantum platform for studying magnetism exemplifies the practical application of these emerging technologies. Future research in quantum computing for modeling physical systems should focus on several key areas. Addressing scalability and error correction is crucial, as creating quantum systems capable of simulating largescale physical models requires overcoming obstacles related to qubit coherence, gate accuracy, and fault-tolerance methods. Research into topological qubits and resilient manipulation techniques is crucial for developing reliable quantum simulators. Furthermore, advancing algorithm development is crucial, particularly quantum algorithms designed for physics simulation, such as those based on quantum imaginary time evolution, which can enhance the modeling of open quantum systems and dynamical phenomena. Integrating hybrid quantum-classical frameworks can leverage the strengths of both approaches to more efficiently simulate complex systems. Application-specific simulations, such as those modeling quantum many-body interactions or unconventional phases of matter, can provide valuable insights and facilitate the creation of specialized quantum simulators. Finally, establishing standardized benchmarking protocols for quantum simulators will promote

consistent and trustworthy results, enhance confidence within the scientific and industrial communities, and encourage wider adoption of these technologies.

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