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Qubits and Superposition: The Quantum Building Block of Computation

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Abstract: Quantum computing exploits quantum mechanical principles to perform computations unachievable by classical systems. Coherent superpositions of states enable quantum parallelism and interference supported by the qubit, the basic unit of quantum computing. This work examines the role of qubits and superposition in quantum information that processes through theoretical foundations and visual simulations. Core formalisms for single-qubit systems are presented, including Dirac notation, unitary and Hermitian , and state evolution. With particular attention to the Hadamard gate for generating and reversing superpositions. The Bloch sphere provides a geometric framework to illustrate the action of single-qubit gates. Qiskit simulations in Python are used to visualise the influence of global and relative phases on qubit dynamics. Physical qubit implementations such as superconducting circuits, trapped ions, and photonic systems are briefly surveyed for context. A practical contribution is the application of the Variational Quantum Eigensolver (VQE) to simulate the dissociation curve of the hydrogen molecule (H_2) and demonstrate the usefulness of hybrid quantum-classical methods for molecular energy calculations in near-term devices. This study highlights the central importance of accurate phase manipulation and single-qubit control in advancing quantum computing by linking mathematical structure, simulation, and application.

Keywords: Quantum Computing, Qubits, Qiskit, Quantum Gates, Variational Quantum Eigensolver

I. Introduction

Classical computers have revolutionised modern life by using binary data strings of bits representing 0s and 1s – and well-defined algorithms to solve problems. However, as issues get more complicated, particularly in domains like simulation, optimisation, and

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cryptography, the constraints of traditional computation become more apparent. A radically novel method for processing information that is not possible with classical systems is provided by quantum computing, which makes use of the ideas of quantum physics [1], [3].

The foundation of quantum computing is the notion that calculations can be carried out using quantum mechanical systems. This idea comes from the discovery that classical computers have trouble effectively simulating quantum processes, which was made most famously by physicist Richard Feynman in the 1980s [1] - [3]. A machine that follows quantum principles could more realistically and effectively simulate such systems if nature is fundamentally quantum. As a result, quantum computing was created.

John Archibald Wheeler, a theoretical physicist, made a substantial contribution to the conceptualisation of quantum information at about the same period. He coined the expression "It from Bit," implying that information is at the core of reality. The philosophical and scientific significance of quantum information [2] was framed by Wheeler's vision of a cosmos in which information and observation are crucial, which further accelerated the development of the science of quantum computation.

A quantum bit or qubit is the central framework and the basic building block of quantum information. In contrast to a classical bit, which can be in only one of two separate states of 0 or 1, a qubit can be in a superposition of both states $|0\rangle$ and $|1\rangle$ at the same time. Mathematically, this superposition is represented as

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Where the complex probability amplitudes α and β satisfy the normalisation condition

$$|\alpha|^2 + |\beta|^2 = 1$$

When a measurement is taken, the qubit "collapses" into one of the basis states – either $|0\rangle$ or $|1\rangle$ – with probabilities governed by the squared values of its complex amplitudes.

Due to the principle of superposition, a quantum computer can handle various possibilities at the same time. This effect, called quantum parallelism, enables a quantum system to assess all possible inputs in a single computational step – an operation that a classical system must perform sequentially [3][8], one input at a time.

However, superposition is not the only source of quantum computation's potency. It also occurs when precisely planned actions, frequently carried out by quantum gates, cause superposed states to interfere with one another. The fundamental principle of many quantum algorithms is the ability to use the concept of interference to cancel out wrong results and enhance accurate ones.

The practical effects of quantum computing go beyond the theoretical concepts and impact various sectors such as artificial intelligence, chemistry, and research on advanced materials [23]. By combining quantum algorithms with the quicker data processing offers with machine learning techniques, Quantum Machine Learning (QML), enhanced optimisation and greater predictive accuracy. In material science, quantum simulations especially utilising algorithms like the Variational Quantum Eigensolver (VQE) allow for the examination of molecular interactions at an unprecedented quantum scale, as demonstrated in the H₂ molecule simulation with Qiskit. At the same time, major industry players like Google, Amazon, and Microsoft are creating unique quantum architectures aimed at achieving scalable, fault-tolerant computing. Collectively, these advancements signify the merging of theory, simulation, and practical application representing a crucial development in the quest for quantum-enhanced technologies [7], [25].

II. Quantum Mechanics

Understanding quantum mechanical processes can be difficult because they deviate from our common experiences based on conventional physics. This paper does not aim to give a comprehensive discussion of quantum mechanics, which takes years of study and specialised training to fully grasp. Rather, its objective is to present the fundamental concepts and mathematical instruments required to comprehend the fundamentals of quantum machines [1] - [3].

A strict set of postulates governs the mathematical theory of quantum mechanics. The behaviour and evolution of quantum systems are defined by these postulates. But from a classical standpoint, the consequences of these axioms frequently produce outcomes that appear contradictory [1], [3]. The Einstein–Podolsky–Rosen (EPR) enigma raises the prospect of instantaneous interactions between distant particles seemingly defying the speed

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of light limitation, while the Compton effect might give the impression that an effect happens before its source.

The quantum mechanical predictions have been very accurately verified through experimentation, even though many of the predictions are contrary to intuition. However, these confirmations frequently require intricate experimental setups and extremely sensitive equipment. This paper starts by concentrating on the theoretical underpinnings and simplified examples of quantum behaviour directly related to quantum computation to introduce the topic.

A. Unitary Matrices

If a matrix U meets the following criteria, it is considered unitary:

$$U^\dagger U = U U^\dagger = I$$

Where:

U^\dagger is the Hermitian adjoint, or conjugate transpose of U .

I is the identity matrix.

The total probability or norm of quantum states remains constant through unitary operations, which are essential to quantum computing. Meaning, when a unitary operator U acts on a quantum state $|\psi\rangle$, the resulting state $U|\psi\rangle$ remains a valid quantum state, and the total probability remains at 1. Quantum gates, which work reversibly on qubits, are shown as unitary matrices [1], [3], [5]. For example, consider:

- Hadamard Gate

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

- Pauli X gate (quantum NOT gate)

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

In quantum calculations, both are unitary matrices used to control qubit states.

B. Hermitian Matrices

If a matrix H equals its conjugate transpose, it is said to be Hermitian:

$$H = H^\dagger$$

In quantum physics, observable quantities like energy, spin, and location are represented by Hermitian matrices, which make them significant. The potential results of a measurement on a quantum system are equivalent to the eigenvalues of a Hermitian operator [3], [5].

For instance, the Pauli-Z matrix or Z gate is Hermitian:

$$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

This matrix is beneficial for describing quantum measurements and phase shifts because it is both Hermitian and unitary.

C. Eigenvectors and EigenValues in Quantum Mechanics

In linear algebra, a non-zero vector that only undergoes a scalar factor change upon application to a matrix A is known as an eigenvector $|\psi\rangle$:

$$A|\psi\rangle = \lambda|\psi\rangle$$

The equivalent eigenvalue in this case is λ .

In quantum mechanics:

- The states that a system may projective measurement into when measured are represented by the eigenvectors of a Hermitian matrix.
- The measured results are called eigenvalues.

For instance, if a Hermitian matrix H represents the observable associated with energy, then measuring the system may yield any of H 's eigenvalues, and the system will collapse into the corresponding eigenvector.

Measurement will reveal one of the eigenvalues with a probability dependent on the squared amplitude of the component along that eigenvector if a quantum system is in a superposition of eigenstates of some observable. This relationship is the foundation of the Born rule [1] - [3].

III. Photon Polarisation

Photon Polarisation provides a convenient physical realisation of a two-level quantum system and serves as an intuitive analogue for qubit superposition.

In quantum mechanics, the polarisation state of a photon is represented as a superposition of two orthogonal basis states, typically chosen as horizontal $|H\rangle$ and vertical $|V\rangle$ polarisation.

The idea of photon polarisation provides one of the easiest means of seeing and comprehending quantum activity. Polarisation provides a mathematically and physically demonstrable representation of several fundamental aspects of quantum mechanics, such as superposition, measurement, and state collapse [1], [2], [15].

The polarisation state of a photon, $|\psi\rangle$, can be mathematically represented as follows:

$$|\psi\rangle = \alpha|H\rangle + \beta|V\rangle$$

where complex values α and β are such that:

$$|\alpha|^2 + |\beta|^2 = 1$$

This example illustrates core quantum features superposition, measurement collapse, and non-classical probabilities in a physically accessible way.

IV. Dirac Notations and the Representation of Qubits

In Quantum computing, quantum states are represented using Dirac (bra–ket) notation within a two-dimensional complex Hilbert space [1], [3]. The computational basis states of a single qubit are expressed as

$$|0\rangle \equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix}, |1\rangle \equiv \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

The basic states $|0\rangle$ and $|1\rangle$ are superposed to form an arbitrary qubit state $|\psi\rangle$:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

Where $\alpha, \beta \in \mathbb{C}$ satisfies the normalisation condition

$$|\alpha|^2 + |\beta|^2 = 1$$

In matrix form, the qubit state is written as

$$|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

V. Representing A Qubit on the Bloch Sphere

The Bloch sphere provides a geometric representation of pure single-qubit states, where each state corresponds to a point on the surface of a unit sphere in three-dimensional space [1], [3].

In this representation, the computational basis states $|0\rangle$ and $|1\rangle$ are located at the north and south poles of the Bloch sphere.

$$|0\rangle \leftrightarrow (0,0,1), \quad |1\rangle \leftrightarrow (0,0,-1)$$

While superposition states lie on the surface between these extrema. The Bloch sphere is particularly useful for visualising relative phase, which is not apparent from measurement probabilities alone.

An arbitrary pure qubit state may be written as

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$

where θ and ϕ are the polar and azimuthal angles on the Bloch sphere. While the polar angle θ determines the measurement probabilities in the computational basis, the azimuthal angle ϕ encodes the relative phase between the basis states.

Of particular interest are the equatorial states, for which $\theta = \pi/2$. The canonical equatorial superposition states are given by

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$$\begin{aligned} |+\rangle &= \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), & |-\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \\ |i\rangle &= \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle), & |-i\rangle &= \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle) \end{aligned}$$

Although these states show the same measurement probabilities in the computational basis, they represent different points on the equator of the Bloch sphere, differing only in their relative phase, ϕ . This difference emphasises the importance of the phase in quantum systems.

The Bloch sphere representation is insensitive to global phase factors, as states of the form $e^{i\gamma}|\psi\rangle$ map to the same point on the sphere. However, relative phase differences cause noticeable effects during unitary evolution. As a result, single-qubit quantum gates can be seen as rotations on the Bloch sphere. Operations like the Hadamard and phase gates perform clear rotations between the poles and the equatorial plane. This geometric view connects the algebraic description of qubit states to their manipulation in quantum circuits.

VI. Manipulating A Qubit – The X, Y, and Z Gates

Single-qubit quantum gates that act on the two-dimensional Hilbert space of a qubit are represented by unitary operators. The Pauli gates X , Y , and Z are the most fundamental among the gates. They form a basis for single-qubit operations and play a central role in quantum algorithms [3], [5]. The Pauli operators are defined as

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The X gate exchanges the computational basis states, mapping $|0\rangle \leftrightarrow |1\rangle$, and corresponds to a rotation by π about the x -axis of the Bloch sphere. The Y gate similarly performs a π -rotation about the y -axis, altering both amplitude and relative phase. The Z gate leaves $|0\rangle$ unchanged while introducing a relative phase shift of π to $|1\rangle$, corresponding to a rotation about the z -axis.

Unlike classical logic gates, Pauli gates can modify the phase of a qubit state without changing measurement probabilities. This distinction is crucial for quantum interference and underpins the behaviour of more complex quantum operations. In the Bloch sphere representation, the action of these gates is naturally interpreted as rigid rotations of the state vector, providing a geometric understanding of qubit manipulation. These rotational

properties form the foundation for composite gates such as the Hadamard and phase gates, which are discussed in the subsequent section.

VII. Introduction to Global and Relative Phase

A qubit may undergo rotations about the Bloch sphere's Z-axis, which correspond to phase transformations and play a fundamental role in quantum computation. Complex numbers which are frequently written in exponential form are reintroduced in quantum computing to quantitatively characterise phase [1], [3], [5].

Complex exponentials provide a concise and understandable means of representing rotations or circular motion, which is why they are employed in quantum computing. For instance, the $|1\rangle$ component of a qubit state can be rotated by ϕ radians about the z-axis by altering the phase angle ϕ in an exponential.

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \rightarrow \alpha|0\rangle + \beta e^{i\phi}|1\rangle$$

The phase angle (ϕ) rotates the $|1\rangle$ component around the z-axis. A rotation of ϕ radians is represented by the complex exponential $e^{i\phi}$. A Phase gate $R_z(\phi)$ Or Z-rotation usually applies to this.

$$R_z(\phi) = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix}$$

A global phase can be factored out, and the relative phase—the quantity of actual interest in quantum operations—is isolated if both the $|0\rangle$ and $|1\rangle$ components have complex coefficients.

$$|\psi\rangle = e^{i\gamma}(\alpha|0\rangle + \beta|1\rangle)$$

The global phase factor $e^{i\gamma}$ has no physical consequences and does not affect measurement probabilities physically. The state is therefore physically equivalent to:

$$|\psi'\rangle = \alpha|0\rangle + \beta|1\rangle$$

Thus $|\psi'\rangle$ represents the physically equivalent state after removal of the global phase.

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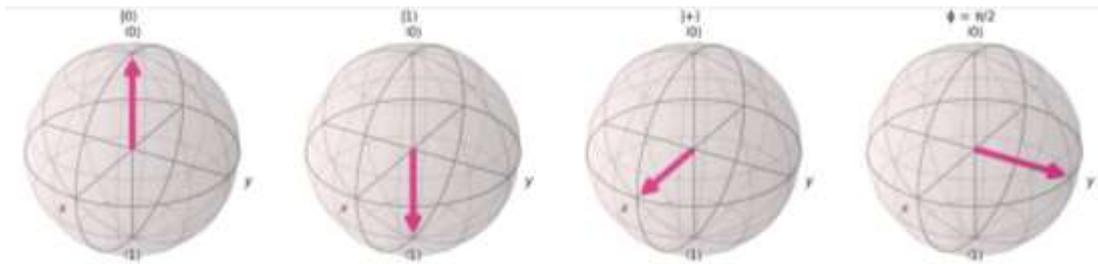


Figure 1: illustrates representative Bloch sphere visualisations of the computational basis states $|0\rangle$ and $|1\rangle$, as well as superposition states $|+\rangle$ and $(|0\rangle + i|1\rangle)/\sqrt{2}$, highlighting the geometric effect of relative phase.

VIII. The Hadamard Gate and $|+\rangle, |-\rangle, |i\rangle$ and $|-i\rangle$ States

The Hadamard gate plays a central role in generating and manipulating equatorial superposition states on the Bloch sphere, which differ only by relative phase while yielding identical measurement probabilities.

On the equator, the four canonical states are:

$$|+\rangle = \left(\frac{1}{\sqrt{2}}\right)(|0\rangle + |1\rangle), \quad |-\rangle = \left(\frac{1}{\sqrt{2}}\right)(|0\rangle - |1\rangle),$$

$$|i\rangle = \left(\frac{1}{\sqrt{2}}\right)(|0\rangle + i|1\rangle), \quad |-i\rangle = \left(\frac{1}{\sqrt{2}}\right)(|0\rangle - i|1\rangle).$$

These states are frequently employed in quantum circuits and quantum information protocols because of their symmetrical placement and orthogonality on the Bloch sphere, making them more than merely mathematical oddities [1][3][5].

The Hadamard gate is self-inverse $H^2 = I$, mapping $|+\rangle \rightarrow |0\rangle$ and $|-\rangle \rightarrow |1\rangle$.

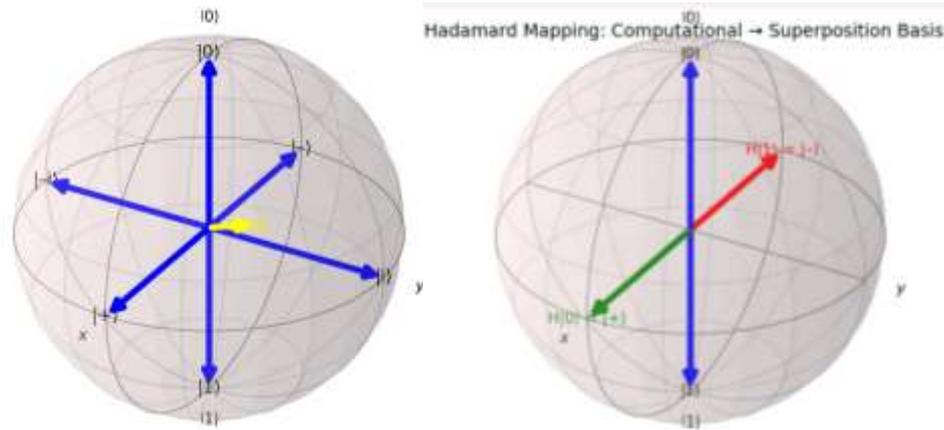


Figure 2 The left figure shows Bloch Sphere visualisation of Hadamard gate transformations and equatorial superposition states. The figure shows $|+\rangle$, $|-\rangle$, $|i\rangle$, and $|-i\rangle$ states, each resulting from Hadamard and phase gate operations. While all states yield equal measurement probabilities, they differ in relative phase. Right figure shows Bloch Sphere visualisation of Hadamard gate transformations between the computational basis ($|0\rangle$, $|1\rangle$) and the superposition basis ($|+\rangle$, $|-\rangle$). The diagram shows how the Hadamard gate maps $|0\rangle$ to $|+\rangle$ and $|1\rangle$ to $|-\rangle$, and vice versa. Generated using Qiskit.

To comprehend the Hadamard gate's phase sensitivity, look at a general qubit state that is

$$|\psi\rangle = \alpha|0\rangle + e^{i\phi}\beta|1\rangle$$

$$H|\psi\rangle = \alpha H|0\rangle + e^{i\phi}\beta H|1\rangle$$

Applying the Hadamard gate yields:

$$= \frac{\alpha + e^{i\phi}\beta}{\sqrt{2}}|0\rangle + \frac{\alpha - e^{i\phi}\beta}{\sqrt{2}}|1\rangle$$

This expression shows how the relative phase ϕ has a major impact on the final state following the use of the Hadamard gate. This shows that states with identical measurement probabilities can evolve differently under the Hadamard gate due to phase-dependent quantum interference.

This demonstrates that the Hadamard gate processes relative phase in addition to amplitude, converting phase information into observable interference. This property is fundamental to quantum algorithms, where computational advantage arises from controlled phase manipulation rather than classical probability alone.

IX. Quantum Processors and Qubit Counts in the Real World

As quantum computing transitions from theoretical constructs to physical implementations, technology leaders such as Google and IBM have developed operational quantum processors based primarily on superconducting qubit architectures. While qubit count is often used as a headline metric, practical quantum performance is equally dependent on qubit fidelity, coherence time, connectivity, and error rates [6]–[8].

A. Google's Quantum Processors

Google's superconducting quantum processors include Bristlecone (72 qubits), designed primarily for scalability testing, and Sycamore (53 qubits), which in 2019 demonstrated a task-specific quantum computational advantage over classical supercomputers [7]. This experiment highlighted the feasibility of executing complex quantum circuits, though it did not represent general-purpose quantum computation.

B. IBM's Quantum Processors

IBM has pursued a systematic roadmap toward scalable quantum computing, introducing processors such as Hummingbird (65 qubits), Eagle (127 qubits), and Heron (133 qubits), all accessible through the IBM Quantum platform [6]. To move beyond raw qubit counts, IBM proposed **Quantum Volume**, a holistic performance metric incorporating qubit number, gate fidelity, connectivity, and circuit depth, providing a more realistic assessment of a quantum processor's computational capability [6], [24].

These developments illustrate that progress in quantum computing depends not only on increasing qubit counts but also on improving qubit quality and system-level reliability.

X. The Creation of Qubits and Their Physical Realisation

Qubits are the basic units of quantum information. They can be created using different quantum systems that show superposition and entanglement. Unlike classical bits made with transistors, qubits need specially designed environments to maintain quantum coherence. This section gives a brief overview of the main physical platforms used in modern quantum processors [1]–[3].

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A. Superconducting Qubits

Superconducting qubits are made using microfabricated superconducting circuits, usually with niobium Josephson junctions or aluminium. In a dilution refrigerator, circuits operate at millikelvin temperature. The thermal noise decreases at these low temperatures, and distinct energy levels appear that allow qubit encoding. Quantum gates are used with precisely controlled microwave pulses. This platform offers fast gate times and scalability, making it the dominant technology used by companies such as Google and IBM [3], [6], [7].

B. Trapped Ion Qubits

Trapped ion qubits encode quantum information in the internal electronic states of ions confined by electromagnetic fields in ultra-high vacuum. Laser-based techniques are used for cooling, state preparation, gate operations, and readout. Although gate speeds are slower than those of superconducting systems, trapped ions exhibit exceptionally high fidelity and long coherence times. This architecture is actively developed by organisations such as IonQ and Honeywell [3], [8].

C. Spin Qubits in Quantum DOTS

Spin qubits utilise the spin states of single electrons confined within semiconductor quantum dots. Control is achieved using gate voltages and magnetic fields, with qubit states represented by spin-up and spin-down configurations. Their compatibility with CMOS fabrication makes spin qubits promising for large-scale integration, though coherence and uniformity remain active research challenges [2], [3].

D. Photonic Qubits

Photonic qubits are very resistant to decoherence and can work at room temperature. Photonic qubits store information as properties like polarisation, phase, or path of individual photons, which makes them ideal for quantum communication and networking. However, generating and entangling photons at scale is still difficult. Companies like PsiQuantum and Xanadu are working on photonic quantum computing designs [3].

XI. The Application of Quantum Computing in Artificial Intelligence: A Potential Future

As artificial intelligence becomes more complex, traditional computational resources limit tasks like optimisation, high-dimensional data analysis, and model training. A potential way to tackle some of these issues is offered by quantum computing by making use of superposition, entanglement, and quantum parallelism [8]–[10].

Quantum Machine Learning (QML) seeks to combine quantum algorithms with classical learning methods. Where proposed quantum versions of techniques such as support vector machines, principal component analysis, and variational learning models [9]–[11]. While theoretical results show possible benefits for certain problem types, practical advantages are still held back by current hardware limits.

Quantum-enhanced optimisation methods like variational quantum algorithms and quantum annealing may improve training and decision making tasks that are basic to AI systems, especially for complex or non-convex problems [8], [9]. However, most QML algorithms remain in the early stages of development and need testing on near-term noisy quantum devices.

For future areas of research, the blend of quantum computing and AI is promising, despite these obstacles. Ongoing improvements in qubit quality, error reduction, and hybrid quantum-classical algorithms will be crucial in determining whether significant benefits over traditional AI systems can be achieved.

XII. Practical Application: Quantum Computing for Material Science

Quantum computing has become an effective instrument for addressing challenges in chemistry and materials science that are beyond the capabilities of classical computers. The behaviour of molecules and materials is determined by the Schrödinger equation, which increases exponentially with the number of particles involved. Conventional computational techniques, such as Density Functional Theory (DFT) and Coupled Cluster approximations, become unmanageable for larger systems because of their computational complexity.

In contrast, quantum computers are capable of directly simulating the dynamics of quantum systems, offering exponential speed advantages for specific applications in chemistry and

materials science [23]. This capability makes them well-suited for estimating molecular energies, mapping reaction pathways, and developing new superconducting or catalytic materials [20], [21].

A. Variational Quantum Eigensolver (VQE)

The Variational Quantum Eigensolver (VQE) is one of the most commonly used hybrid quantum-classical algorithms for determining the ground-state energies of molecules. It integrates the variational principle from quantum mechanics with quantum circuits that generate trial wavefunctions, along with a classical optimiser that aims to minimise the expectation value of the Hamiltonian [4], [20], [22].

The objective is to reduce the following mathematically:

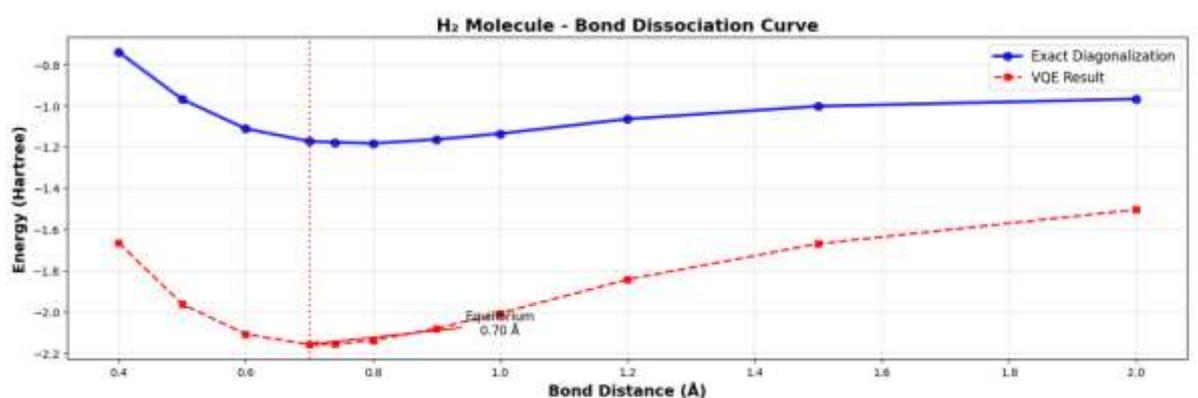
$$E(\theta) = \langle \Psi(\theta) | H | \Psi(\theta) \rangle$$

The molecular Hamiltonian is represented by H , and the state that is parameterised is denoted as $|\Psi(\theta)\rangle$.

In the Qiskit Nature library, the Variational Quantum Eigensolver (VQE) is implemented to enable users to construct Hamiltonians for molecules such as Hydrogen (H_2), Lithium Hydride (LiH), and Beryllium Hydride (BeH_2), which can be solved on both simulators and actual IBM Quantum devices [24].

B. Simulation of H_2 Molecule Using QISKIT

In this study, we utilised Qiskit Nature to simulate the hydrogen molecule (H_2) employing the VQE algorithm [24]. The molecular Hamiltonian was obtained using the STO-3G minimal basis set.



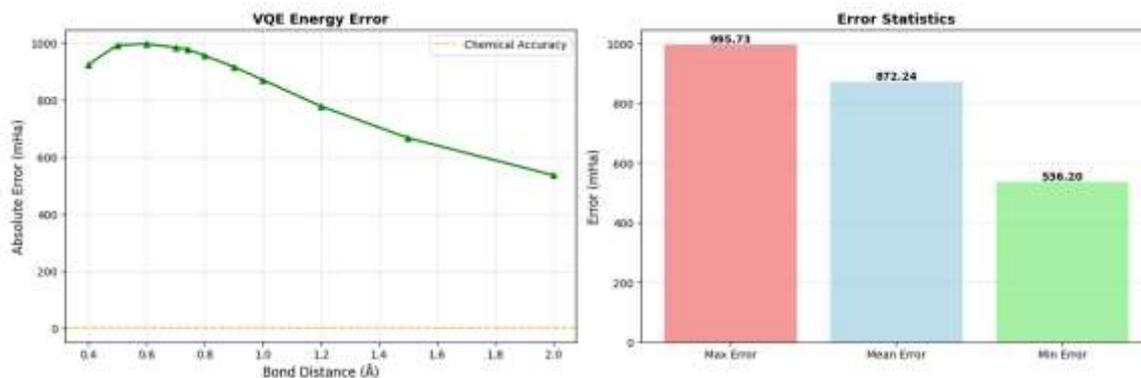


Figure 4: Convergence of the ground-state energy for the H₂ molecule using VQE.

All simulations discussed in this section were carried out using Qiskit 1.x in a Jupyter Notebook environment:

<https://github.com/aditya5ingh7019/H2-Molecule-VQE-Simulation>

We conducted a simulation of the hydrogen molecule (H₂) utilising Qiskit Nature alongside the Variational Quantum Eigensolver (VQE) algorithm. The molecular Hamiltonian was obtained through the STO-3G minimal basis set. To investigate the behaviour of bond dissociation, VQE computations were performed for 11 distinct H–H bond distances varying from 0.40 Å to 2.00 Å.

The findings demonstrate that the VQE algorithm effectively reflects the qualitative behaviour of H₂ dissociation [22]. As the bond distance increases, the absolute errors diminish, underscoring the constraints of the minimal STO-3G basis set and the variational ansatz employed.

A graphical representation displaying the VQE and exact energies in relation to bond distance is provided in Figure 4, depicting the dissociation curve of H₂ along with the associated discrepancies of the VQE results from precise calculations.

C. Results and Energy Estimation

The results of the simulation show that quantum algorithms, including VQE, can effectively calculate the ground-state energy of basic molecular systems with just a limited number of qubits [21]. The convergence graph (Figure 4) illustrates the iterative optimisation process that occurs between quantum and classical elements. As the complexity of the molecules

increases, it is necessary for both the number of qubits and the circuit depth to scale up, highlighting the need for advancements in quantum hardware [23].

D. Implications for Chemistry and Material Science

Quantum computing holds the promise of revolutionising material design, catalyst creation, and drug development [23]. By effectively simulating molecular interactions, scientists can more efficiently create superconducting materials, cryogenic substances, and energy-saving storage systems. Future research will aim to scale these algorithms for larger molecules and incorporate error correction and noise reduction techniques to improve accuracy on near-term quantum processors [24].

XIII. The Rise of Quantum Computing and Its Industrial Advancements

Quantum computing, with major technology companies developing prototype quantum processors based on different architectural philosophies, has progressed from a primarily theoretical discipline to an experimental and industrial research field. Large-scale practical quantum computation remains restrained by decoherence and operational errors, which necessitate robust quantum error correction (QEC) schemes, despite all these advances [13], [14].

Current quantum hardware typically exhibits gate error rates on the order of 10^{-3} to 10^{-2} , exceeding the thresholds required for fault-tolerant computation [13]. Significant industrial effort as a result is directed toward reducing physical error rates and implementing logical qubits capable of sustained error correction.

Different industrial approaches emphasise complementary strategies. While alternative architectures explore hardware-level noise resilience to reduce correction overhead [7], [9]. Superconducting platforms focus on scaling qubit counts and implementing surface-code-based error correction. Although such approaches remain under active investigation, Experimental research into topologically protected qubits aims to achieve intrinsic robustness against decoherence [7], [26].

These developments highlight that the central challenge in quantum computing is not merely increasing qubit numbers, error-resistant qubits capable of supporting long quantum computations, but achieving stability. Control precision will ultimately determine the

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viability of quantum computing for real-world applications and continued progress in error correction, materials engineering, and control.

XIV. Challenges, Readiness, and The Future of Quantum Computation

Although advancements in quantum hardware are progressing expeditiously, quantum software development remains a significant congestion [9]. Quantum processors inherently produce probabilistic outputs that must be interpreted using carefully designed algorithms [21]. Present error-correcting codes and noise-mitigation techniques are still insufficient for reliable performance across diverse problem classes, resulting in most current demonstrations being proof of concept rather than commercially deployable systems [23], [25].

The Technology Readiness Level (TRL) framework provides a useful metric for assessing progress [25]. At present, most quantum computing technologies remain within TRL 3–4, corresponding to laboratory validation stages. However, expert assessments indicate cautious optimism that higher readiness levels may be achieved within the next decade, contingent on sustained advances in hardware, algorithms, and error correction [25].

The implementation of fault-tolerant error correction schemes, scalable qubit fabrication with acceptable noise levels, and core challenges include the development of quantum algorithms that outperform classical methods in practical applications, and the establishment of a skilled quantum workforce capable of operating and advancing these systems [7], [20], [21], [23], [25]. Foremost, quantum computers are expected to complement rather than replace classical systems, particularly for problems such as molecular simulation, optimisation, and cryptographic analysis [12], [23].

XV. Final Conclusion Exploiting superposition, entanglement, and quantum interference, quantum computing distinctly departs from classic computing due to its unique methodologies. The qubit is the foundation of quantum computing because it is able to remain in a coherent superposition and allows for computations that cannot be achieved with classical computing systems. In this paper, I will describe how quantum state evolution is determined by the quantum gate operation (Hadamard), representations of the Bloch sphere, and unitary operations and subsequently show how these are the distinguishing points between quantum logic and classical information processing.

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Experiments on actual physical implementations of qubits such as superconducting circuits, trapped ions, photonic systems, and spin-based architectures all present alternative experimental methodologies for developing scalable and fault-tolerant quantum hardware; however, all research on quantum computing is limited by, but not limited to decoherence, noise, and overhead costs of error correcting codes and will place the majority of systems within the earlier technology readiness phase.

At present, we are in the process of moving quantum computing from theory into practice through continued improvement of qubit stability, application of various algorithms, and other forms of error mitigation that will determine one aspect of how quantum computing will play out as an emerging field. Thus, in addition to generally being an addition to performing tasks on a desktop, quantum computing systems will be operating with classical computing systems, performing very specialised tasks that are impossible to complete using classical computing methods.

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