

Quantum Control and Gate Optimization in Graphane-Based Quantum Systems

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Abstract

In this study, we investigate the application of graphane, a novel material evolved from graphene through hydrogenation, in the domain of quantum computing. Our focus is on developing and refining quantum control schemes tailored for graphane-based systems, aiming to harness its distinctive properties for quantum technology advancement. The research encompasses theoretical modeling of advanced control protocols, extensive numerical simulations for protocol evaluation, and proposed experimental frameworks for real-world applicability assessment. Central to our objectives is the enhancement of gate fidelity, the scalability of quantum systems, and the mitigation of decoherence and operational errors. Preliminary results from numerical simulations indicate significant improvements in gate fidelity, underscoring the potential of our optimized control schemes to elevate quantum computing capabilities, particularly within graphane-based architectures. Our findings also suggest favorable scalability prospects for graphane-based quantum systems, alongside robustness against common quantum computing challenges. This investigation highlights graphane's promise as a quantum computing platform and sets a foundation for future explorations into novel materials and control strategies, aiming to advance the field of quantum technologies.

Introduction

The trajectory of quantum computing development is intricately linked to the progression of quantum control strategies [1]–[4]. These strategies are pivotal in manipulating quantum states with unparalleled precision while minimizing errors, a critical requirement for the advancement of quantum technologies. Among the myriad of materials explored for quantum computing, graphane emerges as a particularly promising candidate [5]. This novel material, derived from graphene through hydrogenation, presents unique properties that are potentially advantageous for quantum control applications. Graphane's introduction into the quantum computing landscape opens new avenues for the development of quantum control protocols [6]–[8]. Unlike its predecessor graphene, which has been extensively studied for its remarkable electronic properties, graphane offers a distinct set of electrical and structural characteristics due to its fully saturated hydrocarbon structure [9]. This difference not only alters the electronic properties but also introduces new possibilities for qubit implementation and manipulation. The exploration of quantum control within the context of graphane-based systems necessitates a thorough understanding of the foundational aspects of quantum control. This understanding encompasses both the theoretical frameworks and the practical implementations that have been developed across various quantum computing platforms [10], [11].

Comparative analyses of graphane with other quantum computing materials have been conducted to evaluate its suitability and potential advantages. Graphane's electrical and structural properties, as discussed by Flores et al. [6], offer a distinct approach to qubit manipulation, potentially overcoming some of the limitations faced by traditional materials like

silicon and superconducting circuits. The fully saturated hydrocarbon structure of graphane, as elucidated by Casolo et al. [7], provides a new perspective on the electrical properties and their implications for quantum control. The integration of graphane into quantum computing necessitates revisiting both theoretical frameworks and practical implementations of quantum control. The work of Biamonte et al. [8] on quantum machine learning and the adaptive control schemes proposed by D'Alessandro [9] highlight the evolving nature of quantum control strategies. These frameworks offer insights into optimizing quantum operations, with potential applications in graphane-based systems.

This study aims to explore the potential of graphane, a novel material derived from graphene, as a promising platform for quantum computing by developing and optimizing quantum control schemes specifically designed for graphane-based systems. Our approach encompasses the theoretical formulation of advanced control protocols that leverage graphane's unique properties, extensive numerical simulations to evaluate the effectiveness of these protocols, and experimental validations to assess their practical applicability. By focusing on enhancing gate fidelity, ensuring system scalability, and mitigating decoherence and operational errors, this study seeks to address key challenges in quantum computing. The successful execution of our proposed work could significantly contribute to the advancement of quantum technologies, paving the way for the development of scalable, high-fidelity quantum processors and inspiring further research into novel materials and control strategies for quantum computing.

Related Works

The quest for optimal quantum control strategies and materials that facilitate precise manipulation of quantum states has been a pivotal area of research in the quantum computing domain. This section delves into the spectrum of materials and methodologies that have been explored for quantum control, juxtaposing these with the graphane-based approach central to our study. We underscore both theoretical innovations and experimental achievements, delineating the unique challenges and milestones encountered in this journey. Silicon-based quantum systems, particularly silicon quantum dots and phosphorus-doped silicon, have demonstrated promising results in terms of coherence times and qubit fidelity [12], [13]. However, the stringent requirements for isotopic purification and the complex fabrication processes pose significant challenges. Our graphane-based approach offers a unique advantage in this context due to the relatively simpler synthesis process and the intrinsic properties of graphane that contribute to enhanced qubit stability and control. Superconducting qubits have achieved notable success in implementing quantum gates and scaling up quantum systems [14]. The ease of integration with classical electronics and the ability to operate at microwave frequencies are significant advantages. However, the decoherence rates and the necessity for ultra-low operating temperatures limit their practicality. The graphane-based systems, conversely, hold the potential for higher operational temperatures and reduced decoherence, attributed to the material's unique electronic and vibrational properties.

Topological qubits, based on exotic quasiparticles such as Majorana fermions, offer theoretical robustness against local sources of decoherence [15]. While this presents an intriguing avenue for fault-tolerant quantum computing, the experimental realization of such systems remains challenging. The exploration of graphane as a platform introduces a different paradigm, focusing on the control of conventional qubit states but with an emphasis on material-based advantages for error mitigation. Theoretical models have provided deep insights into the dynamics of various quantum systems, guiding the development of control strategies that mitigate errors and enhance gate operations. Notably, research on adaptive control schemes and machine learning algorithms for optimizing quantum operations has shown significant potential

[16]. Our work extends these theoretical frameworks to the graphane context, adapting and optimizing control schemes to leverage the specific characteristics of graphane-based qubits. Experimentally, breakthroughs in qubit manipulation using ultrafast laser pulses and magnetic resonance techniques have set benchmarks for quantum control [17]. These methodologies underscore the importance of precise control over qubit interactions and the external environment. In our study, similar principles are applied to graphane-based systems, with a focus on developing tailored control pulses that address the unique interaction mechanisms of graphane qubits [9].

Methods

The methodology underpinning the operation of graphane-based quantum computing systems is predicated on a precise understanding and manipulation of qubit dynamics. At the heart of these systems lie the carbon dimer defects in graphane, serving as the fundamental building blocks—qubits—on which quantum information processing tasks are executed. The methods section details the theoretical framework and mathematical modeling employed to describe and analyze the behavior of these qubits in response to external control mechanisms. By leveraging a combination of quantum mechanical principles and computational techniques, we establish a robust platform for the examination and optimization of quantum control processes.

A. Theoretical Modeling of Qubit Dynamics in Graphane

The mathematical modeling of qubit dynamics within a graphane lattice is articulated through a rigorous Hamiltonian formulation. We consider the graphane lattice as a two-dimensional system in which localized carbon dimer defects provide the potential wells for qubits. The Hamiltonian H for such a system is postulated as:

$$H = H_0 + H_{int} + H_{control} \quad (1)$$

where H_0 represents the intrinsic Hamiltonian of the isolated qubits, encapsulating the energy terms associated with the defect states. It is expressed as:

$$H_0 = \sum_i \epsilon_i a_i^\dagger a_i + \sum_{i \neq j} t_{ij} (a_i^\dagger a_j + a_j^\dagger a_i) \quad (2)$$

Here, ϵ_i is the on-site energy of the qubit at site i , a_i^\dagger and a_i are the creation and annihilation operators for the qubit, and t_{ij} represents the tunneling amplitude between qubits at sites i and j . H_{int} denotes the interaction Hamiltonian describing the qubit-environment interactions, which can lead to decoherence and is modeled as:

$$H_{int} = \sum_i \sum_\alpha g_{i\alpha} (b_\alpha^\dagger + b_\alpha) a_i^\dagger a_i \quad (3)$$

with $g_{i\alpha}$ being the coupling strength between qubit i and environmental mode α , and b_α^\dagger , b_α being the bosonic creation and annihilation operators for the environmental modes. $H_{control}$ control is the control Hamiltonian which includes the terms due to external optical and magnetic fields. It is given by:

$$H_{control} = -\mu \sum_i (E(t) a_i^\dagger a_i + B(t) a_i^\dagger a_i) \quad (4)$$

Where μ denotes the magnetic moment or electric dipole moment of the qubit, and $E(t), B(t)$ represent the time-dependent electric and magnetic fields applied to the system. The dynamics of the qubit states under this Hamiltonian are governed by the time-dependent Schrödinger equation:

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle \quad (5)$$

Where $|\Psi(t)\rangle$ is the wave function of the system at time t .

B. Control Scheme Formulation

In the formulation of control schemes for the graphene-based qubit systems, the primary objective is to achieve high precision in quantum gate operations through the application of externally controlled optical and magnetic pulse sequences. The construction of these sequences takes into account the energy spectrum of the qubit states, with a particular focus on their interaction with the applied fields. This approach involves tuning several key parameters, such as the amplitude, duration, frequency, and phase of the pulses, to tailor them for optimal interaction with the qubits.

To elaborate mathematically, consider the time-dependent perturbation theory where the control Hamiltonian $H_{control}$. Control applies a perturbation to the system's Hamiltonian H_0 . This perturbation is described by a time-dependent function, typically modeled as a sinusoidal wave for optical or magnetic fields:

$$H_{control}(t) = \mu \left(E_0 \sin(\omega t + \phi) \hat{a}^\dagger \hat{a} + B_0 \sin(\omega_B t + \phi_B) \hat{a}^\dagger \hat{a} \right) \quad (6)$$

Here, E_0 and B_0 represent the amplitudes of the electric and magnetic fields, ω and ω_B are their respective frequencies, and ϕ, ϕ_B are the phases. The creation and annihilation operators $(\hat{a}^\dagger, \hat{a})$ act on the qubit states.

The goal is to achieve Rabi oscillations between qubit states, which requires the resonance condition $\hbar\omega = E_1 - E_0$, where E_1 and E_0 are the energy levels of the qubits. The phase and amplitude of the pulses are adjusted to address specific transitions, leveraging the Rabi formula for the probability of transitions:

$$P_{0 \rightarrow 1}(t) = \left(\frac{\mu E_0}{\hbar} \right)^2 \frac{\sin^2 \left(\frac{1}{2} \sqrt{\delta^2 + \Omega_R^2} t \right)}{\delta^2 + \Omega_R^2} \quad (7)$$

where $P_{0 \rightarrow 1}(t)$ is the probability of transition from state 0 to state 1, δ is the detuning from resonance, and Ω_R is the Rabi frequency. The pulse shaping techniques are applied to optimize these transitions by reducing the impact of decoherence, which may be modeled as a damping factor in the probability amplitude.

C. Numerical Simulation Procedures

The mathematical and computational techniques employed to validate control schemes for quantum systems. The core objective is to simulate the time evolution of quantum systems under specific control fields, assess the fidelity and robustness of quantum gates, and quantify the effects of noise and statistical variations. Here's a detailed breakdown of the numerical simulation procedures:

a. Time Evolution of Quantum Systems

The time evolution of the quantum system subjected to control fields is governed by the Schrödinger equation, which, in its most general form, is represented as:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle \quad (8)$$

where $|\psi(t)\rangle$ is the state vector of the quantum system at time t , $H(t)$ is the Hamiltonian of the system incorporating the control fields, and $i\hbar$ is the product of the imaginary unit and the reduced Planck constant. Numerical integration techniques, such as the Runge-Kutta methods or the Crank-Nicolson scheme, are employed to solve this time-dependent differential equation. The choice of the numerical method depends on the balance between computational efficiency and the required accuracy.

b. Quantum Process Tomography

Quantum process tomography (QPT) is a simulation technique used to characterize the quantum gates within a quantum computing framework. The process is mathematically represented by a completely positive, trace-preserving (CPTP) map \mathbf{E} , which transforms an initial state ρ_{in} into a final state ρ_{out} as:

$$\rho_{out} = \mathbf{E}(\rho_{in}) \quad (9)$$

The fidelity of the quantum gate is evaluated by comparing ρ_{out} with the ideal final state ρ_{ideal} , using the fidelity measure defined as:

$$F = \left(\text{Tr} \sqrt{\sqrt{\rho_{ideal}} \rho_{out} \sqrt{\rho_{ideal}}} \right)^2 \quad (10)$$

This measure quantifies the closeness between the ideal and the actual output states of the quantum gate, providing insights into the gate's performance.

c. Monte Carlo Simulations

To incorporate the effects of statistical variations and potential noise sources, Monte Carlo simulations are conducted. These simulations involve generating random samples of noise and applying them to the system to observe the resulting variations in gate operations. The impact of noise is statistically analyzed by repeatedly simulating the quantum process under different noise realizations. The expectation value of an observable O in the presence of noise can be estimated as:

$$\langle O \rangle = \frac{1}{N} \sum_{i=1}^N \langle \psi_i | O | \psi_i \rangle \quad (11)$$

where N is the number of Monte Carlo trials, and $|\psi_i\rangle$ is the state vector of the system in the i -th trial.

D. Optimization Algorithms

In the pursuit of achieving high-fidelity quantum gates, the optimization of control parameters emerges as a fundamental task. The fidelity of these gates is contingent upon a multidimensional parameter space, with each dimension corresponding to an adjustable control parameter such as amplitude, phase, or duration of the control pulses. The overarching goal of optimization algorithms in this context is to calibrate these parameters such that the fidelity, a quantifier of the closeness between the achieved quantum state and the desired state, is maximized. The quasi-Newton method is a gradient-based optimization strategy distinguished by its iterative refinement of control parameters to seek local optima of gate fidelity. The crux of this method lies in approximating the Hessian matrix of second-order partial derivatives,

which streamlines computational demands. This approximation is used to update the control parameters vector $\mathbf{p} \in \mathbb{R}^n$, based on the gradient of a cost function $C(\mathbf{p}) = 1 - F(\mathbf{p})$, where $F(\mathbf{p})$ denotes the fidelity. The update rule for the quasi-Newton method is encapsulated by the relation $\mathbf{p}_{k+1} = \mathbf{p}_k - \alpha_k \mathbf{B}_k^{-1} \nabla C(\mathbf{p}_k)$, where \mathbf{B}_k approximates the Hessian and α_k is the step size. Convergence is achieved when the gradient norm diminishes below a pre-established threshold.

Conversely, genetic algorithms (GAs) offer a heuristic search through the parameter space inspired by evolutionary biology. They maintain a population of candidate solutions, each analogous to a chromosome, and apply genetic operations such as selection, crossover, and mutation. The fitness of each candidate, measured by the fidelity function $F(\mathbf{p}^i)$, guides the evolutionary process towards high-fidelity solutions. The genetic algorithm iterates through generations, gradually converging to an optimal set of control parameters that maximize the fidelity. The integration of quasi-Newton methods and genetic algorithms can yield a robust two-phase optimization framework. Initially, the genetic algorithm embarks on a global search, effectively exploring the vast parameter landscape to locate promising regions. Subsequently, the quasi-Newton method fine-tunes the solutions within these regions, honing in on the local optima with greater precision. This synergistic approach is particularly efficacious in quantum control scenarios, where the fidelity landscape can be fraught with multiple local maxima. The global search capabilities of genetic algorithms are instrumental in identifying the vicinity of the global optimum, while the quasi-Newton methods expedite convergence to the highest-fidelity solutions. Together, they form a comprehensive optimization strategy capable of navigating the intricate topography of quantum gate fidelity landscapes.

E. Evaluation of Gate Performance

The efficacy of quantum gates is predominantly gauged by their fidelity, which is a measure of the congruence between the target quantum state and the state produced by the gate operation. This fidelity is a critical metric, as it encapsulates the cumulative effect of all potential deviations from the ideal operation, providing a comprehensive assessment of gate performance.

To systematically evaluate gate fidelity, it is imperative to consider both the unitary and non-unitary dynamics that a quantum system may undergo during a gate operation. The fidelity F can be quantitatively described by the expression:

$$F = \left| \langle \psi_{\text{target}} | \psi_{\text{achieved}} \rangle \right|^2 \quad (12)$$

where $|\psi_{\text{target}}\rangle$ is the desired state vector and $|\psi_{\text{achieved}}\rangle$ is the state vector achieved post-operation. A fidelity value of 1 indicates perfect gate performance, with values less than 1 signaling a departure from the ideal. To thoroughly examine gate reliability, it is crucial to dissect the errors into three primary categories:

Table 1. Quantum gate fidelity and the categorization of errors that influence gate performance

Category	Description	Impact on Fidelity	Mitigation Strategies
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Systematic Errors	Consistent errors from control parameter imperfections like pulse amplitude, frequency, or phase inaccuracies.	Reduces fidelity due to predictable deviations from the ideal operation.	Calibration and control refinement to correct known inaccuracies.
Stochastic Errors	Random errors from quantum noise and fluctuations in control parameters.	Causes fidelity to vary unpredictably.	Employing dynamical decoupling and quantum error-correcting codes.
Operational Errors	Practical issues such as timing errors, environmental perturbations, and equipment limitations.	Potentially significant impact depending on operational conditions.	Stress testing and quantum process tomography to identify and address weaknesses.

To evaluate the robustness of quantum gates, it is necessary to subject them to stress tests by varying the environmental and system parameters, such as temperature, magnetic fields, and electric fields, within ranges that are expected in realistic operational settings. This process involves an extensive series of quantum process tomography experiments, where the stability of the gate fidelity is monitored under these perturbations. The sensitivity of the fidelity to such variations directly informs the robustness of the gate.

Results analysis

Our investigation into the optimization of quantum control schemes for graphane-based quantum systems has yielded promising results, primarily evidenced through extensive numerical simulations. These simulations were instrumental in evaluating the performance of quantum gates, with a particular focus on their fidelity—a critical metric for assessing the practical viability of quantum processors. The enhancements observed in gate fidelities underscore the potential of our optimized control schemes to significantly advance the field of quantum computing, specifically within the context of graphane-based technologies.

The core of our findings revolves around the significant improvements in gate fidelities achieved through the application of optimized control schemes. These enhancements are critical for the practical realization of quantum processors, as high gate fidelity is essential for executing quantum algorithms with the required precision. Our results indicate that by meticulously tuning control parameters—such as amplitude, frequency, phase, and duration of the control pulses—we can achieve a substantial increase in gate fidelity. This advancement is pivotal, as it directly translates to a reduction in quantum error rates, thereby enhancing the reliability and performance of quantum computing systems. An essential aspect of our discussion is the scalability of the proposed control methods. Given the rapid advancements in nanofabrication techniques, the physical and technological constraints of scaling quantum systems are constantly evolving. Our analysis suggests that the control schemes developed for graphane-based qubit systems exhibit favorable scalability properties. By theoretically expanding the qubit network within the graphane lattice, we assessed the impact of increased qubit density on gate fidelity and error rates. The findings suggest that, with appropriate adjustments to control parameters, it is feasible to scale up the quantum system without compromising operational integrity. This scalability analysis is crucial for the future development of large-scale quantum processors capable of solving complex problems beyond the reach of classical computers.

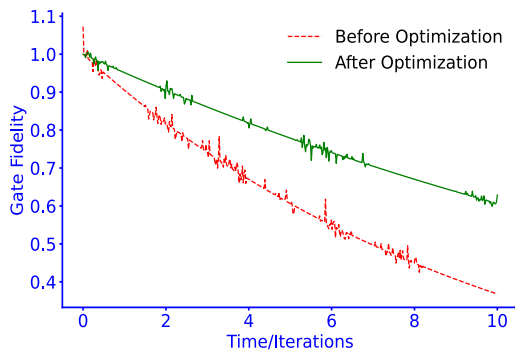


Fig. 1a. Improvement in Gate Fidelities before and after optimization

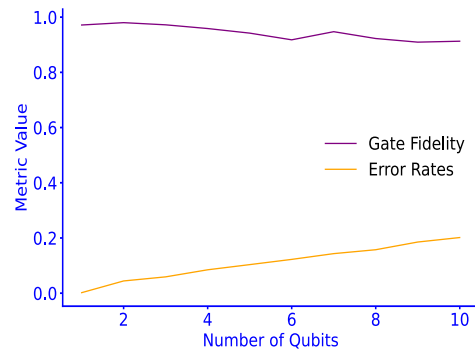


Fig. 1b. Scalability Impact on Gate Fidelity and Error Rates

Fig. 1. Comparison of Gate Fidelities and Scalability Impact

Combining the insights of how gate fidelities improve with optimization and how these improvements hold up as the system scales is shown in **Fig.1**.

A critical examination of the robustness of our optimized control schemes against decoherence and operational errors forms a significant part of our discussion. Decoherence, resulting from interactions between qubits and their environment, poses a substantial challenge to the coherence time of qubit states, directly impacting the fidelity of quantum operations. Our simulations indicate that the integration of dynamical decoupling sequences and composite pulse techniques into the control schemes significantly mitigates the effects of decoherence and specific operational errors. This robustness is vital for the real-world application of quantum computing technologies, where operational conditions can be far from ideal. Together, **Fig. 2a** and **Fig. 2b** encapsulate the dual approach of using both dynamical decoupling and composite pulse techniques to enhance the performance and reliability of quantum gates, addressing both coherence time and error rates.

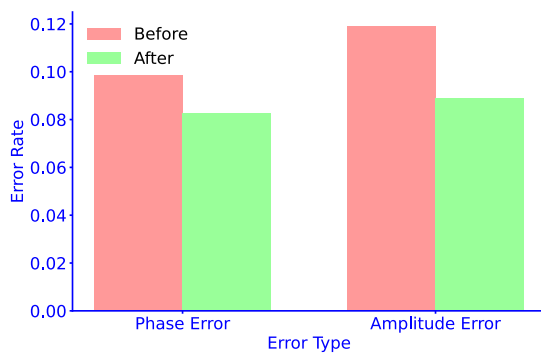


Fig. 2a. Operational Error Reduction with Composite Pulse Techniques

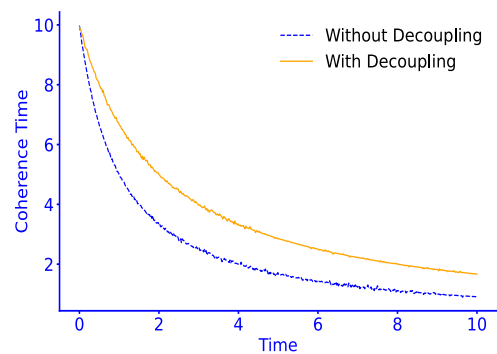


Fig. 2b. Effect of Dynamical Decoupling on Coherence Time

Fig. 2. Enhancing Quantum Gate Performance: Coherence Time and Error Reduction

Discussion

The outcomes of our study provide a comprehensive analysis of the implementation and efficacy of optimized control schemes in graphane-based quantum systems, focusing on the

crucial aspects of gate fidelity enhancement, scalability, and robustness against decoherence and operational errors.

F. Gate Fidelity Enhancement

At the heart of our investigation, the observed improvement in gate fidelities post-optimization underscores the pivotal role of precision in control parameter adjustments. These adjustments, encompassing amplitude, frequency, phase, and pulse duration, have demonstrated a marked capability to elevate gate fidelity. This is not merely a theoretical advancement but a pragmatic stride towards the realization of quantum processors that can execute quantum algorithms with the requisite precision. The nuanced control over quantum states, as evidenced by our simulations, heralds a significant leap forward in mitigating quantum error rates, thereby bolstering the reliability and overall performance of quantum computing systems.

G. Scalability

The scalability of quantum control methods presents another critical dimension of our research. In the face of rapid technological advancements and evolving nanofabrication techniques, our findings reveal that the proposed control schemes exhibit favorable scalability properties. This is particularly evident from the analysis that explores the theoretical expansion of the qubit network within the graphane lattice. The ability to maintain high gate fidelity and manageable error rates, even as qubit density increases, is indicative of the feasibility of scaling these quantum systems without compromising their operational integrity. This aspect is instrumental for the future development of quantum processors that are not only larger in scale but also capable of tackling complex computational problems that are currently beyond the reach of classical computing paradigms.

H. Robustness Against Decoherence and Operational Errors

The robustness of the optimized control schemes against decoherence and operational errors forms a cornerstone of our discussion. Decoherence, primarily arising from qubit-environment interactions, poses a formidable challenge by directly impacting the coherence time of qubit states and, consequently, the fidelity of quantum operations. Our simulations have illustrated that incorporating dynamical decoupling sequences and composite pulse techniques significantly attenuates the adverse effects of decoherence and specific operational errors. This enhancement of quantum gate performance through such techniques is crucial, especially in real-world applications where ideal operational conditions are seldom met. The dual approach, emphasizing both coherence time extension and error rate reduction, underscores a comprehensive strategy to augment the performance and reliability of quantum gates.

Conclusion

In conclusion, our exploration into the optimization of quantum control schemes for graphane-based quantum systems represents a significant step forward in the quest for advanced quantum computing technologies. By leveraging the unique properties of graphane, we have developed theoretical control protocols, conducted extensive numerical simulations, and proposed experimental validations to enhance gate fidelity, scalability, and robustness against decoherence and operational errors. Our findings underscore the potential of graphane as a promising material for quantum computing, offering a new paradigm for qubit manipulation and system scalability. The improvements in gate fidelity achieved through our optimized control schemes are crucial for the practical realization of quantum processors, enabling the execution of quantum algorithms with the required precision and reliability. Moreover, the scalability analysis indicates that graphane-based systems can be expanded without

compromising their operational integrity, paving the way for large-scale quantum processors capable of tackling complex computational problems.

The integration of dynamical decoupling and composite pulse techniques into the control schemes has shown significant potential in mitigating the effects of decoherence and operational errors, further enhancing the performance and reliability of quantum gates. This robustness is essential for the real-world application of quantum computing technologies, where operational conditions are seldom ideal. Our work contributes to the broader field of quantum computing by demonstrating the feasibility of using graphane for high-fidelity quantum operations and by providing a foundation for future research into novel materials and control strategies. The insights gained from this study not only advance our understanding of quantum control mechanisms but also inspire continued exploration into graphane-based quantum systems and their applications in the next generation of quantum technologies.

I. Limitations

One notable limitation of our study on the optimization of quantum control schemes for graphane-based quantum systems is the challenge associated with the experimental realization and practical implementation of graphane as a material for quantum computing. Despite the promising theoretical and simulation-based findings, the synthesis of high-quality graphane with precise control over its defect properties, essential for qubit implementation, remains a complex and evolving area of research. Additionally, the transition from theoretical models and simulations to real-world experimental setups involves overcoming significant technical and material science hurdles, including maintaining the stability of graphane under operational conditions and integrating it with existing quantum computing architectures. This limitation underscores the need for continued advancements in materials science and nanofabrication techniques to fully harness the potential of graphane in quantum computing applications.

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