Variational Quantum Algorithms via Measurement-Induced Passive Steering

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***Abstract*—Variational quantum algorithms (VQA) combine the advantages of classical and near-term quantum computation for solving problems on today's noisy quantum devices. Variational Quantum Eigensolver (VQE) is one of the widely used VQAs, which aims to find the approximate ground state energy of a given Hamiltonian. While traditional VQE implementation is promising for ansatz-based trial state preparation, it requires an initial fiducial state or a reference state, which can be infeasible for large quantum systems. In this paper, we propose a novel approach for trial state preparation in VQE algorithms. This method leverages passive steering, a circuit-based approach with repeated measurements, eliminating the need for an initial fiducial state or a reference state. Experimental results demonstrate that passive steering-based state preparation provides improved accuracy and scalability of VQE compared to traditional ansatz-based solutions. Our proposed solution can also be effectively combined with the existing ansatz-based methods, where passive steering prepares the reference state while ansatz prepares the trial state, facilitating a robust and scalable state preparation for variational quantum algorithms.**

***Index Terms*—Quantum Computing, Variational Quantum Algorithms, Variational Quantum Eigensolver, Ansatz, State Preparation, Passive Steering**

I. Introduction

Quantum computers use the unique features of quantum states, such as superposition, entanglement, and interference, to perform calculations faster than classical computers, introducing new possibilities for solving a certain class of problems that are hard for classical computers. Despite these advances, quantum computing is still an emerging field, facing challenges such as noise, error rates, the stability of quantum bits (qubits), and difficulty in building large quantum systems. Noisy Intermediate-Scale Quantum (NISQ) computers [1], [2], though limited by their noise levels and the number of qubits, offer a platform to explore quantum computing applications on a scale previously unattainable. The development of NISQ technology marks a critical step in quantum research, acknowledging the current limitations while laying the groundwork for future advancements.

Variational quantum algorithms (VQA) [3], [4], [5], [6] enable the synergistic integration of classical and quantum computing to effectively navigate challenges like noise and the limited scale of current quantum computers. Specifically, variational quantum algorithms, such as Variational Quantum Eigensolver (VQE) [7], [8], [9], harness the precise control and optimization capabilities of classical computing alongside the parallel processing power and quantum state manipulation offered by quantum computing. VQE has shown remarkable promise in addressing complex problems in various domains, including quantum chemistry [10], [11], [8] and materials science [9], [12]. By utilizing quantum computers to estimate the eigenvalues of a Hamiltonian, VQE leverages the unique ability of quantum systems to represent, manipulate, and process information in ways that classical systems cannot. This capability, combined with classical computers' power to manage optimization routines, forms a potent method for solving problems beyond the reach of current classical computers.

While existing VQE-based solutions are promising, they face two fundamental challenges. First, the presence of short coherence times, system noise, and frequent gate errors in NISQ computers [1] complicate the execution of larger-scale experiments due to the challenges in accurately implementing state preparation circuits. Moreover, the existing VQE frameworks depend on the choice of the reference state and the ansatz parameters [13]. A well-chosen reference state can accelerate the VQE process by narrowing the search space. However, identifying an optimal reference state is challenging, and preparing it assumes the existence of a known fiducial state ($|0\rangle^{\otimes n}$of n-qubits), which is difficult to achieve in larger quantum systems [14].

In this paper, we address the fundamental challenge of state preparation in variational quantum algorithms. Specifically, we propose a passive steering-based [14] ansatz designed to outperform widely used Qiskit's [15] ansatz-based solutions, such as Unitary Coupled Cluster Singles and Doubles (UCCSD) [16] and hardware efficient SU(2) 2-local circuit (EfficientSU2) [17], especially in large noisy quantum environments with unknown initial state. Unlike existing ansatz-based methods that rely on a reference state or initial known state to construct the trial state, our approach eliminates the need for such prerequisites. Our approach can generate the quantum circuit required to produce the desired trial state using measurement-induced passive steering. This represents a significant departure from traditional ansatzes, where the trial state is adjusted by tuning parameters within a fixed circuit structure. In contrast, our method focuses on directly shaping the trial state itself, subsequently deriving the circuit through passive steering mechanisms to produce this state. Specifically, this paper makes the following major contributions.

- We propose a passive steering-based trial state preparation method, thereby eliminating the initial state dependency in VQE algorithms. Experimental results demonstrate that passive steering-based state preparation provides improved accuracy and scalability of VQE compared to traditional ansatz-based solutions.
- We also demonstrate an effective combination of passive steering with the traditional ansatz, where passive steering prepares the reference state while ansatz prepares the trial state, facilitating a robust and scalable state preparation for variational quantum algorithms.

The remainder of this paper is organized as follows: Section II provides the necessary background on VQE and passive steering. Section III describes our passive steering-based state preparation framework, aiming to replace the traditional ansatz and reference state preparation circuit in VQE. Section IV presents the experimental results. Finally, Section V concludes the paper.

II. Background and Related Work

A. Varitional Quantum Eigensolver

Eigensolvers are used to find the eigenvalues and eigenvectors of a system [18]. It enables the discovery of ground state energies of Hamiltonians crucial in quantum chemistry, advanced simulations in nuclear physics, and aids in the design of quantum algorithms for optimization problems. These tools are also significant in material science [19], [20] for identifying new materials with desired properties and in cryptography for efficiently factoring large numbers. However, classical eigensolvers, which typically involve operations like matrix diagonalization, face significant limitations due to the exponential scaling of computational resources with system size. This makes it impractical to analyze large or complex quantum systems as the computational demand far exceeds the capabilities of classical computing infrastructure.

In order to address these limitations, VQE implementations utilize a hybrid quantum-classical approach by leveraging the strengths of quantum and classical computers to approximate the minimum eigenvalue (ground state energy) [8]. VQE operates by preparing a trial quantum state, measuring observables to evaluate its energy, and employing classical optimization to adjust the trial state's parameters toward minimizing its energy. This method capitalizes on quantum computers' ability to handle complex quantum state manipulations and classical computers' optimization capabilities.

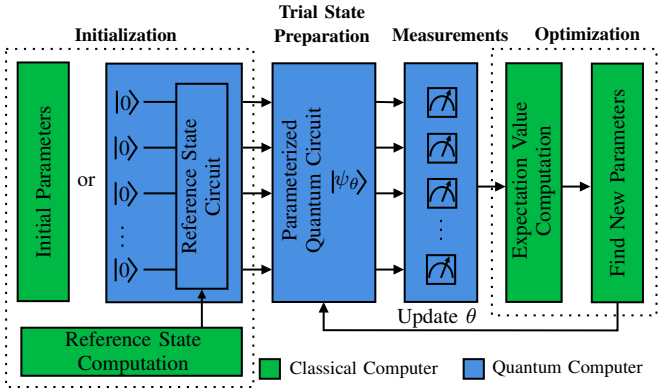


Fig. 1: Traditional VQE consists of four stages: initialization, trial state preparation, measurement, and optimization. The computations are divided between classical and quantum computers, as shown by green and blue colors, respectively.

As shown in Figure 1, a traditional VQE framework consists of four stages. The first stage either initializes a reference state, which can be obtained from mean field calculations like the Hartree-Fock method [21] for problems like electronic structures or initializes ansatz parameters by guessing or by using past data. This step is followed by the deployment of a parameterized quantum circuit known as ansatz, such as UCCSD, TwoLocal, EfficientSU2, etc. The choice of ansatz is critical, as it determines the algorithm's capacity to explore the Hilbert space effectively, balancing expressibility and the manageability of the computational search space [3]. The measurement phase of VQE involves applying rotations to align the measurement basis with the system's observables, thus enabling the acquisition of precise energy information of the trial state. This data is then processed by a classical optimizer, like COBYLA [22], to iteratively refine the ansatz parameters towards achieving the lowest energy state. This iterative loop continues until the optimizer converges on a solution, demonstrating the algorithm's efficacy in approximating the ground state energy using NISQ computers.

B. Measurement-Induced Passive Steering

There are various methods for preparing quantum states, such as thermal relaxation and algorithmic cooling to obtain a fiducial state or applying a series of discrete quantum gates to the known initial state to obtain the target state. The existing methods can be inefficient for large quantum systems due to long relaxation times, the complexity of required operations, or the need for careful calibration of quantum gates. Moreover, direct initialization faces with scalability concerns and can introduce unacceptable overhead for large-scale quantum systems. Measurement-induced quantum steering (MIQS) [14], [23] exploits the non-local correlations inherent in quantum mechanics to manipulate the state of a quantum system indirectly. This technique hinges on the establishment of entanglement between the system and an ancillary system, the latter being subjected to measurements that induce a back-action on the system, thus steering it towards the desired state. This iterative protocol leverages the repetition of quantum measurements and unitary transformations to navigate the state space.

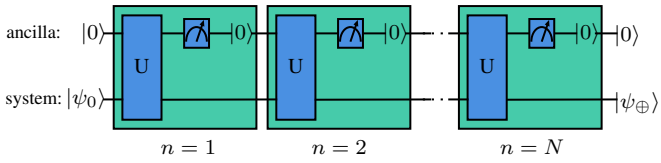


Fig. 2: Illustration of the iterative process for steering an unknown initial state, $|\psi_0\rangle$, towards the designated target state, $|\psi_\oplus\rangle$, after N applications, utilizing passive steering [14].

Figure 2 shows the iterative steps of the MIQS protocol that are outlined as follows:

- A unitary operation U is applied to entangle the system and ancilla qubits, transforming the state of the ancilla-system after the n^{th} iteration $\rho^{n+1}_{\text{ancilla}-\text{system}} = U(\rho_{\text{ancilla}} \otimes \rho^{n}_{\text{system}})U^\dagger$, where ρ_{ancilla} represents the density matrices of the ancilla and ρ^{n}_{system} represents the density matrices of the system after n iterations.

The selected U should satisfy the steering inequality: $\langle\psi_{\oplus}|\rho^{n}_{\text{system}}|\psi_{\oplus}\rangle < \langle\psi_{\oplus}|\rho^{n+1}_{\text{system}}|\psi_{\oplus}\rangle$.

- The measurement of ancilla qubits leads to the state of the system conditioned on the measurement outcome of the ancilla. The system's state after measurement is given by $\rho^{n+1}_{\text{system}} = Tr_{\text{ancilla}}[\rho^{n+1}_{\text{ancilla-system}}]$, where $\text{Tr}_{\text{ancilla}}$ is the trace of ρ_{ancilla}.
- Following the measurement, the ancilla qubits are reset to their initial state for the next iteration, making the process memory-less. This protocol incrementally steers the system towards the target state. Since here we are disregarding the measurement results, this approach is called passive steering.

The MIQS protocol aims to maximize the fidelity of the prepared state, with each iteration bringing the system closer to the desired target state.

III. Passive Steering based State Preparation

The concept of an ansatz plays a pivotal role in the trial state preparation in the VQE framework. An ansatz is essentially a parameterized quantum circuit designed to explore the quantum system's Hilbert space in search of its ground state energy. In this section, we first discuss a hybrid state preparation approach by utilizing both traditional ansatz and passive steering. Next, we discuss passive steering-based trial state preparation as a replacement for the traditional ansatz in the VQE framework.

A. State Preparation using Passive Steering and Ansatz

This section explores an effective combination of passive steering and ansatz, where passive steering prepares the reference state and ansatz prepares the trial state, as outlined in the following sections.

1) Trial State Preparation using Ansatz: The ansatz's purpose within the VQE pipeline is to generate trial states that are iteratively optimized, based on the feedback from quantum measurements, to find the system's ground state energy as closely as possible. Selecting an effective ansatz is crucial for the success of VQE because it directly influences the algorithm's ability to converge to the true ground state within a feasible number of iterations. The main criterion for selecting an ansatz is its expressibility, which refers to the ansatz's capacity to generate a diverse set of states across the Hilbert space. Expressibility can be defined in terms of the Kullback-Leibler divergence that compares the distribution of states generated by the ansatz to a uniform distribution in Hilbert space, also known as the Haar random states. For a given ansatz C, the quantified expressibility $\varepsilon(C)$ is defined as follows in terms of Kullback-Leibler (KL) divergence [24]:

$$\begin{aligned}\varepsilon(C) &= D_{KL}(P(C,F)||P_{\text{Haar}}(F)) \\ &= \int_0^1 P(C,F)\log\left(\frac{P(C,F)}{P_{\text{Haar}}(F)}\right)dF.\end{aligned} \tag{1}$$

where $D_{KL}(p||q)$ is the KL-divergence between probability distributions p and q. $P(C,F)$ is the estimated probability distribution of the fidelity (F), which can be defined as:

$$F = |\langle\psi_{\theta}|\psi_{\phi}\rangle|^2 \tag{2}$$

where θ and ϕ are randomly sampled parameters from the ansatz C. $P_{\text{Haar}}(F)$ is the probability distribution of fidelity F for the Haar random state which is defined as

$$P_{\text{Haar}}(F) = (N-1)(1-F)^{N-2} \tag{3}$$

where N is the dimension of the Hilbert Space. The ansatz C is considered more expressible if it has a lower KL-divergence value with respect to the Haar measure. Hardware-efficient ansatz (EfficientSU2), UCCSD, and heuristic excitation-preserving wave function ansatz (ExcitationPreserving) are prominent examples of different types of ansatz available in the Qiskit environment. These varieties highlight the breadth of strategies developed to navigate the complexities of quantum state preparation, each with its unique approach to balancing expressibility and computational efficiency.

2) Reference State Preparation using Passive Steering: In quantum chemistry, many ansatzes begin with a reference state, typically a product state, derived from mean-field calculations such as Hartree-Fock. These reference state circuits are predicated on the assumption that the initial state of the qubits in the VQE pipeline is a known fiducial state. However, as previously discussed, traditional methods of preparing these known fiducial states can be inefficient in larger quantum systems. By implementing passive steering for reference state preparation, our proposed method circumvents the need for a predetermined fiducial state. Figure 3 depicts how this reference state is prepared via passive steering, which is then integrated with traditional ansatz in the VQE pipeline, demonstrating a combined strategy that boosts both the performance and flexibility of the algorithm.

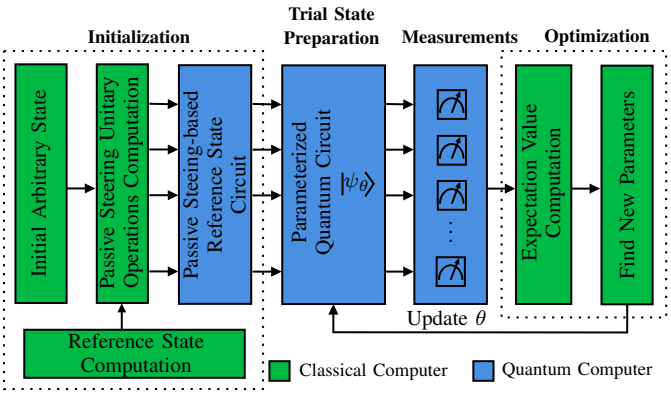


Fig. 3: State preparation using both passive steering and ansatz

B. State Preparation using Passive Steering

In this section, we discuss a solution for state preparation using only passive steering. The passive steering-based trial state preparation avoids the reliance on internal parameterized gates for state generation. Instead, it capitalizes on the principles of MIQS to directly guide the quantum state towards the desired state, acting effectively as a dynamic ansatz. One of the key advantages of passive steering-based state preparation

is that it can achieve any target state starting from any initial state. Therefore, this method is well suited for large quantum systems where state preparation is a challenging task. As shown in Figure 4, our approach allows for the complete replacement of ansatz-based trial state preparation with passive steering within the VQE pipeline. Here, classical optimization is applied not to tune parameterized gates in each iteration but to adjust the parameters of the wave function itself, offering a more direct and more efficient route to state preparation, as demonstrated in Section IV.

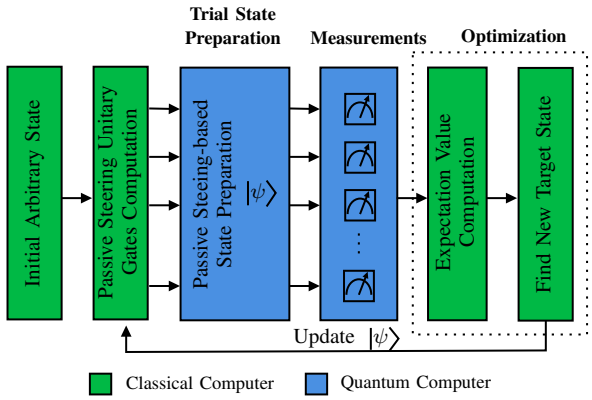


Fig. 4: Proposed passive steering-based VQE framework

IV. Experiments

In this section, we present experimental results to demonstrate the effectiveness of passive steering-based state preparation in the VQE framework.

A. Experimental Setup

We conducted our experiments using the Qiskit [15] simulator. To compare our passive steering-based trial state preparation method against state-of-the-art approaches, we selected a range of inbuilt ansatzes available in Qiskit, including UCCSD [16], EfficientSU2 [17], RealAmplitudes [25], TwoLocal [26], and ExcitationPreserving [27]. To ensure a fair assessment of all ansatzes, we employed the same VQE algorithm implementation, including consistent measurement circuit generation, expected value calculation, and classical optimization techniques across all trials. The COBYLA optimizer, known for its gradient-free approach to optimization, was chosen as the classical optimizer for its robustness in handling the algorithm's non-linear optimization challenges. We utilized the Qiskit Aer simulator [28] with the state vector method as our simulator. All the results were obtained as an average of ten rounds, with each round consisting of 8192 shots. These experiments were executed on a Mac mini with an 8-core Apple M2 processor and 16 GB of RAM.

We focus on computing the ground state energy of the H_2 molecule across a range of interatomic distances and compare our approach with existing methods as well as the exact ground state energy. Specifically, VQE determines the molecule's ground state energy by finding the minimum eigenvalue of its Hamiltonian matrix. To achieve this, we input the Hamiltonian of the H_2 molecule, modified to reflect various interatomic distances, into the VQE and calculate the ground state energy for each distance using different trial state preparation methods. For reference, we employ a mathematical eigenvalue solver (NumpyEigenSolver [29]) to compute the exact ground state energy of the given Hamiltonian.

B. State Preparation Results Utilizing Both Passive Steering and Traditional Ansatz

As described in Section III-A2, passive steering-based state preparation is utilized to generate an initial fiducial state-independent reference state, which is then combined with the UCCSD ansatz to execute the VQE. We utilized the Hartree-Fock method to find the reference state by using classical computation and constructed a passive steering-based circuit to achieve that reference state for the current system's initial state. Figure 5a presents the H_2-based experiment using our proposed combined ansatz (passive steering and UCCSD), with the exact (mathematical) value as the reference. In this experiment, the only UCCSD ansatz was initialized with the Hartree-Fock reference state, while the combined ansatz was also initialized with the same Hartree-Fock reference state but with the passive steering-based circuit. We observed that our proposed approach (combined ansatz) produces results comparable to that of the state-of-the-art (UCCSD).

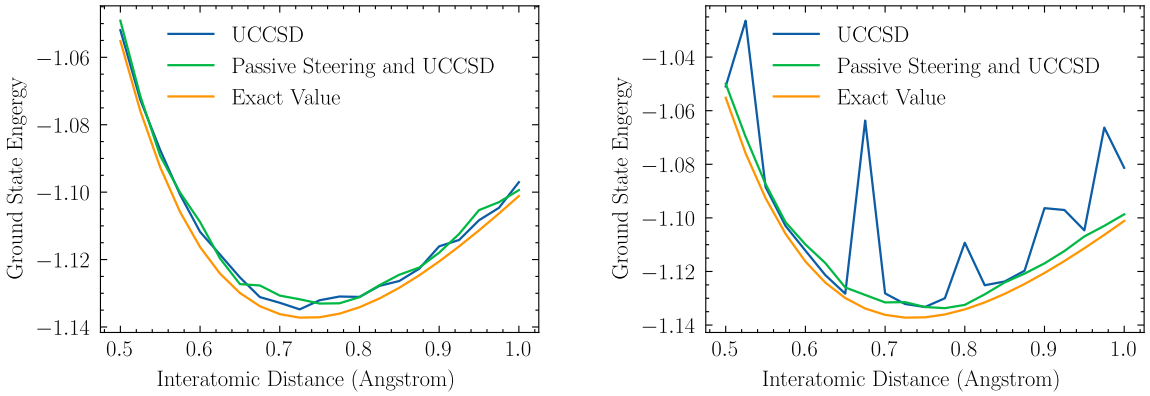
To demonstrate the advantages of the combined ansatz, we conducted the same H_2-based experiment in a noisy environment. We utilized a noise model available in Qiskit to incorporate noise factors such as measurement errors, gate imperfections, and decoherence effects. Figure 5b shows the results of this experiment, which clearly highlight the noise-resilient state preparation capabilities of passive steering, while UCCSD is not stable in a noisy environment.

C. State Preparation Results using Passive Steering

We first evaluate the expressibility of passive steering-based state preparation. Next, we compare our approach (with a random initial state) and traditional ansatz (with a known initial state) in a noise-free environment. We repeat the same experiment with a random initial state for all methods. Finally, we repeat these experiments in a noisy environment.

1) Expressibility of Passive Steering-based State Preparation: In this experiment, we evaluate the expressibility of the passive steering, focusing on how well it can explore quantum states. To visualize this effectively, we use a single qubit to represent states on a Bloch sphere. Figure 6a depicts a Bloch sphere with 4000 uniformly sampled states, generated from 5000 pairs of target states, which are inputs for passive steering-based state preparation.

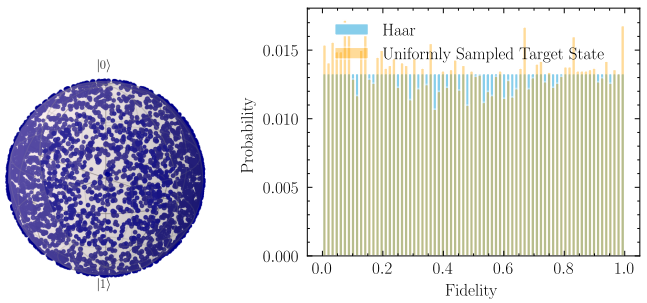
To estimate the probability distribution of the fidelity, $F = |\langle\psi_\theta|\psi_\phi\rangle|^2$, where $|\psi_\theta\rangle$ and $|\psi_\phi\rangle$ are uniformly sampled target states, we employed histograms with a bin number of 75. The distribution is illustrated by the orange histogram in Figure 6b. We compare this with the fidelity distribution for a Haar-distributed ensemble, described by Equation 3 showcased as the blue histogram in the same figure.



(a) Comparison of VQE results without noise

(b) Comparison of VQE Results with noise

Fig. 5: Comparison of H_2 ground state energy produced by our approach (passive steering and UCCSD) and UCCSD.



(a) Passive steering-based uniform state preparation laid with the Haar measure.

(b) Histogram of estimated fidelity over-

Fig. 6: Quantified expressibility for single-qubit circuit

Based on Equation 1, we calculate the KL-divergence for our method as 0.0211, indicating the expressibility of passive steering-based state preparation. The smaller the KL-divergence, the more closely our method's fidelity distribution aligns with that of the ideal Haar measure, suggesting high expressibility. For comparison, we also calculated the KL-divergence for the UCCSD ansatz using the same number of samples, which yields 0.4147. These results highlight that the passive steering can evenly explore quantum state spaces.

2) State Preparation in a Noise-Free Environment: We compare our approach (passive steering with random initial state) against traditional ansatz-based state preparation.

Traditional Ansatz with Known Initial State: Figure 7a illustrates the computed ground state energies at different interatomic distances using VQE with passive steering for state preparation, alongside the results from VQE with UCCSD ansatz and the exact values. Our proposed method can produce results comparable with state-of-the-art (UCCSD).

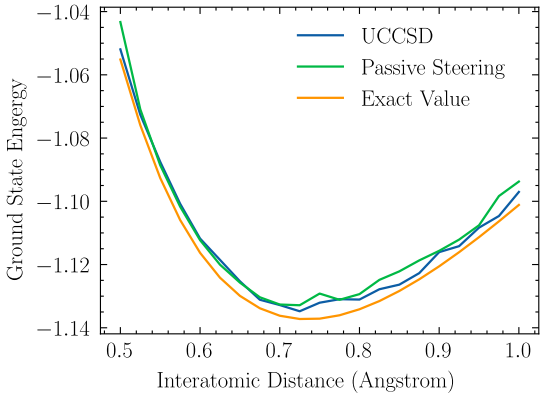
As shown in Figure 7b, we also compare our approach with five widely utilized ansatzes using a box and whisker plot. For ease of illustration, we have used the following acronyms: UCCSD (US), EfficientSU2 (ES), RealAmplitudes (RA), TwoLocal (TL), ExcitationPreserving (EP), and Passive Steering (PS). In this comparison, we compute the logarithmic difference between the ground state energies calculated by VQE and the exact values. In this experiment, every traditional ansatz was initialized with the Hartree-Fock reference state, while a random initial state was used for the passive steering-based preparation. Figure 7b reveals that passive steering achieves results of comparable accuracy to traditional methods, even without relying on a predefined reference state.

Traditional Ansatz with Random Initial State: In this experiment, we initialize all ansatzes with a random state and execute VQE to determine the ground state energy of the H_2 molecule across varying interatomic distances. Figure 8a shows the computed ground state energies at various interatomic distances using VQE with passive steering for state preparation, as well as the results obtained from VQE with the UCCSD ansatz and the exact values. Our proposed method significantly outperforms state-of-the-art (UCCSD) because of its capability of the initial state independent state preparation.

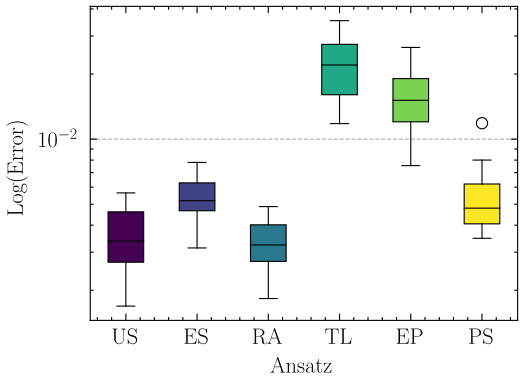
We also computed the error by comparing the VQE results with the exact ground state energy and visualized this error using a box and whisker plot. As depicted in Figure 8b, the passive steering-based method performs equally or better than other ansatzes employed in our study. For instance, the widely used chemistry-inspired UCCSD ansatz is significantly less accurate compared to the passive steering-based trial state preparation, exhibiting nearly tenfold higher median error without a pre-set initial state. While ansatzes such as TwoLocal, EfficientSU2, and RealAmplitude demonstrate comparable results to passive steering, their efficacy cannot be guaranteed for larger quantum systems [30].

3) State Preparation in a Noisy Environment: We have conducted the same two experiments as outlined above under noisy conditions. Specifically, we compare our approach (passive steering with random initial state) with traditional ansatz-based state preparation.

Traditional Ansatz with Known Initial State: Figure 9a presents a box and whisker plot illustrating the error in VQE results for various ansatzes when initialized with a Hartree-Fock reference state, taking into account the effects of noise. We can observe that passive steering-based state preparation achieved comparable results even without an initial state.

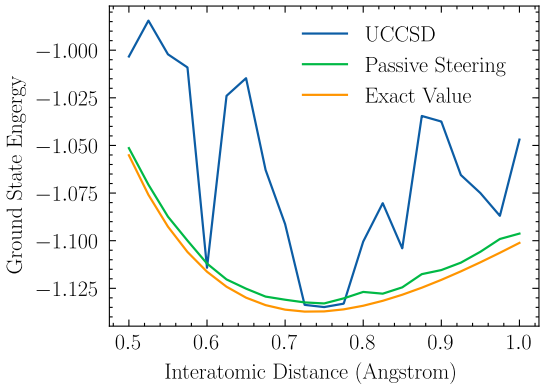


(a) H_2 ground state energy comparison with UCCSD.

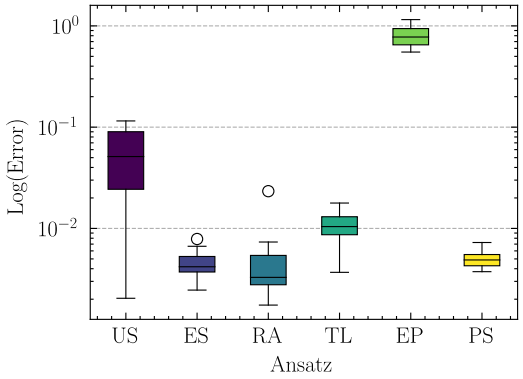


(b) Error comparison with traditional ansatz.

Fig. 7: Comparison of H_2 ground state energy produced by our approach (passive steering with random initial state) and state-of-the-art (five traditional ansatz-based solutions with **known** initial states).

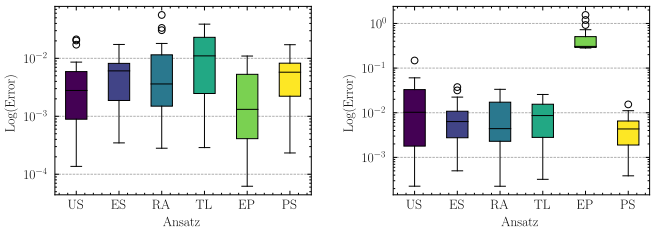


(a) H_2 ground state energy comparison with UCCSD.



(b) Error comparison with traditional ansatz-based.

Fig. 8: Comparison of H_2 ground state energy produced by our approach (passive steering with random initial state) and state-of-the-art (five traditional ansatz-based solutions with **random** initial states).



(a) Comparison with traditional ansatz with **known** initial states

(b) Comparison with traditional ansatz with **random** initial states

Fig. 9: Error comparison of H_2 ground state energy produced by our approach (passive steering with random initial state) and traditional ansatz-based solutions in noisy environments.

Traditional Ansatz with Random Initial States: Figure 9b displays the error in VQE results without the use of a reference state, indicating the performance under noisy conditions with random initial states. We can see that our proposed method outperforms most of the tested ansatzes in a noisy environment with a random initial state. For example, the proposed method is around 2.5-fold more accurate than the UCCSD.

V. Conclusion

Variational quantum eigensolvers (VQE) can effectively utilize the benefits of both classical computers and near-term noisy quantum computers to find the approximate ground state energy of a given Hamiltonian. A fundamental bottleneck in traditional VQE is that it assumes the availability of an initial fiducial state or a reference state, which can be infeasible for large quantum systems. In this paper, we developed a passive steering-based state preparation framework that does not require an initial fiducial state or a reference state. We have also explored an effective combination of passive steering and traditional ansatz. Extensive experimental evaluation demonstrated that our proposed framework can outperform state-of-the-art ansatz-based solutions (UCCSD, EfficientSU2, RealAmplitudes, TwoLocal, and ExcitationPreserving). Our findings highlighted that passive steering-based trial state preparation can significantly enhance the efficiency and accuracy of VQE in quantum computing applications, particularly for large-scale quantum systems, paving the way for developing robust and scalable quantum algorithms.

Acknowledgments

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REFERENCES

[1] J. Preskill, "Quantum computing in the nisq era and beyond," *Quantum*, vol. 2, p. 79, 2018.

[2] D. Volya and P. Mishra, "Impact of noise on quantum algorithms in noisy intermediate-scale quantum systems," in *IEEE International Conference on Computer Design (ICCD)*, 2020.

[3] J. R. McClean, J. Romero, R. Babbush, and A. Aspuru-Guzik, "The theory of variational hybrid quantum-classical algorithms," *New Journal of Physics*, vol. 18, no. 2, p. 023023, 2016.

[4] Y. Li and S. C. Benjamin, "Efficient variational quantum simulator incorporating active error minimization," *Physical Review X*, vol. 7, no. 2, p. 021050, 2017.

[5] M. Lubasch, J. Joo, P. Moinier, M. Kiffner, and D. Jaksch, "Variational quantum algorithms for nonlinear problems," *Physical Review A*, vol. 101, no. 1, p. 010301, 2020.

[6] T. Jones, S. Endo, S. McArdle, X. Yuan, and S. C. Benjamin, "Variational quantum algorithms for discovering hamiltonian spectra," *Physical Review A*, vol. 99, no. 6, p. 062304, 2019.

[7] M.-H. Yung, J. Casanova, A. Mezzacapo, J. Mcclean, L. Lamata, A. Aspuru-Guzik, and E. Solano, "From transistor to trapped-ion computers for quantum chemistry," *Scientific reports*, vol. 4, no. 1, p. 3589, 2014.

[8] A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'brien, "A variational eigenvalue solver on a photonic quantum processor," *Nature communications*, vol. 5, no. 1, 2014.

[9] A. Kandala, A. Mezzacapo, K. Temme, M. Takita, M. Brink, J. M. Chow, and J. M. Gambetta, "Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets," *nature*, vol. 549, no. 7671, pp. 242–246, 2017.

[10] N. C. Rubin, R. Babbush, and J. McClean, "Application of fermionic marginal constraints to hybrid quantum algorithms," *New Journal of Physics*, vol. 20, no. 5, p. 053020, 2018.

[11] Y. Shen, X. Zhang, S. Zhang, J.-N. Zhang, M.-H. Yung, and K. Kim, "Quantum implementation of the unitary coupled cluster for simulating molecular electronic structure," *Physical Review A*, vol. 95, no. 2, p. 020501, 2017.

[12] J. Romero, R. Babbush, J. R. McClean, C. Hempel, P. J. Love, and A. Aspuru-Guzik, "Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz," *Quantum Science and Technology*, vol. 4, no. 1, p. 014008, 2018.

[13] A. Choquette, A. Di Paolo, P. K. Barkoutsos, D. Sénéchal, I. Tavernelli, and A. Blais, "Quantum-optimal-control-inspired ansatz for variational quantum algorithms," *Physical Review Research*, vol. 3, no. 2, p. 023092, 2021.

[14] D. Volya and P. Mishra, "State preparation on quantum computers via quantum steering," *IEEE Transactions on Quantum Engineering*, 2024.

[15] H. Abraham, I. Akhalwaya, G. Aleksandrowicz, T. Alexander, G. Alexandrowics, E. Arbel, A. Asfaw, C. Azaustre, P. AzizNgoueya, G. Barron *et al.*, "Qiskit: an open-source framework for quantum computing. zenodo," 2019.

[16] Q. documentation, "Uccsd," https://docs.quantum.ibm.com/api/qiskit/0.31/qiskit.chemistry.components.variational_forms.UCCSD, accessed: 2024-03-30.

[17] ——, "Efficientsu2," https://docs.quantum.ibm.com/api/qiskit/qiskit.circuit.library.EfficientSU2, accessed: 2024-03-30.

[18] G. H. Golub and H. A. Van der Vorst, "Eigenvalue computation in the 20th century," *Journal of Computational and Applied Mathematics*, vol. 123, no. 1-2, pp. 35–65, 2000.

[19] V. Lordi and J. M. Nichol, "Advances and opportunities in materials science for scalable quantum computing," *MRS Bulletin*, vol. 46, pp. 589–595, 2021.

[20] B. Bauer, D. Wecker, A. J. Millis, M. B. Hastings, and M. Troyer, "Hybrid quantum-classical approach to correlated materials," *Physical Review X*, vol. 6, no. 3, p. 031045, 2016.

[21] J. D. Whitfield, J. Biamonte, and A. Aspuru-Guzik, "Simulation of electronic structure hamiltonians using quantum computers," *Molecular Physics*, vol. 109, no. 5, pp. 735–750, 2011.

[22] M. J. Powell, *A direct search optimization method that models the objective and constraint functions by linear interpolation*. Springer, 1994.

[23] D. Volya, Z. Pan, and P. Mishra, "Feedback-based steering for quantum state preparation," in *IEEE International Conference on Quantum Computing and Engineering (QCE)*, 2023, pp. 1308–1318.

[24] S. Sim, P. D. Johnson, and A. Aspuru-Guzik, "Expressibility and entangling capability of parameterized quantum circuits for hybrid quantum-classical algorithms," *Advanced Quantum Technologies*, vol. 2, no. 12, p. 1900070, 2019.

[25] Q. documentation, "Realamplitudes," https://docs.quantum.ibm.com/api/qiskit/qiskit.circuit.library.RealAmplitudes, accessed: 2024-03-30.

[26] ——, "Twolocal," https://docs.quantum.ibm.com/api/qiskit/qiskit.circuit.library.TwoLocal, accessed: 2024-03-30.

[27] ——, "Excitationpreserving," https://docs.quantum.ibm.com/api/qiskit/qiskit.circuit.library.ExcitationPreserving, accessed: 2024-03-30.

[28] ——, "Aersimulator," https://qiskit.github.io/qiskit-aer/stubs/qiskit_aer.AerSimulator.html, accessed: 2024-03-30.

[29] ——, "Numpyeigensolver," https://docs.quantum.ibm.com/api/qiskit/0.26/qiskit.algorithms.NumPyEigensolver, accessed: 2024-03-30.

[30] Y. Li, J. Hu, X.-M. Zhang, Z. Song, and M.-H. Yung, "Variational quantum simulation for quantum chemistry," *Advanced Theory and Simulations*, vol. 2, no. 4, p. 1800182, 2019.