Variational Quantum Eigensolvers for Molecular Ground-State Estimation: A Benchmark on Noisy Intermediate-Scale Quantum Hardware

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Abstract

The variational quantum eigensolver (VQE) is among the most promising near-term algorithms for estimating molecular ground-state energies on noisy intermediate-scale quantum (NISQ) devices. In this work, we benchmark a hardware-efficient VQE ansatz against a chemistry-inspired unitary coupled-cluster singles and doubles (UCCSD) ansatz for a set of small molecular systems, including hydrogen (H2), lithium hydride (LiH), and beryllium hydride (BeH2). Simulations were performed under realistic noise models calibrated to superconducting qubit hardware, incorporating gate infidelity, T1/T2 decoherence, and readout error. We find that the hardware-efficient ansatz converges faster in gate count but exhibits a systematically higher variance in energy estimates due to barren plateau effects at larger qubit counts, while UCCSD offers better chemical accuracy at the cost of significantly deeper circuits. We further evaluate three error-mitigation strategies -- zero-noise extrapolation, readout-error mitigation, and symmetry verification -- and show that a combination of readout mitigation and zero-noise extrapolation recovers chemical accuracy for H2 and LiH on simulated 7-qubit and 12-qubit devices respectively. Our results offer practical guidance for ansatz and mitigation strategy selection when deploying VQE workloads on current-generation quantum hardware.

1. Introduction

Simulating molecular electronic structure is widely regarded as one of the most promising near-term applications of quantum computing, owing to the exponential scaling of classical methods with system size. The variational quantum eigensolver (Peruzzo et al., 2014) addresses this by combining a parameterized quantum circuit with a classical optimization loop, making it comparatively robust to the depth and coherence limitations of current noisy intermediate-scale quantum (NISQ) devices. Despite this robustness, ansatz choice, optimizer behaviour, and hardware noise all materially affect whether a given VQE implementation reaches chemical accuracy (typically defined as within 1.6 mHa of the exact result) within a practical number of circuit evaluations.

This paper presents a systematic comparison of two commonly used ansatz families under realistic noise, together with an evaluation of standard error-mitigation techniques, with the goal of providing practical guidance to researchers selecting a VQE configuration for near-term hardware experiments.

2. Methods

All simulations were carried out using a statevector and density-matrix noise simulator configured with gate and readout error rates drawn from calibration data typical of superconducting transmon processors. Two ansatz families were tested: a hardware-efficient ansatz composed of alternating single-qubit rotation and entangling layers, and a chemistry-inspired UCCSD ansatz derived from second-quantized fermionic excitation operators via the Jordan-Wigner transformation. The classical optimization loop used the Simultaneous Perturbation Stochastic Approximation (SPSA) optimizer, chosen for its resilience to measurement shot noise relative to gradient-based alternatives.

Three error-mitigation techniques were evaluated in isolation and in combination: zero-noise extrapolation via unitary folding, measurement/readout-error mitigation via calibration matrix inversion, and symmetry verification based on particle-number conservation.

3. Results

For H2 on a minimal STO-3G basis (2 qubits after parity reduction), both ansatz families reached chemical accuracy in the noiseless case. Under simulated hardware noise, the hardware-efficient ansatz showed an average energy error of 4.8 mHa without mitigation, reduced to 1.1 mHa with combined readout mitigation and zero-noise extrapolation. UCCSD, while requiring roughly 2.3 times the two-qubit gate count, showed a smaller unmitigated error of 3.1 mHa, falling to 0.9 mHa under the same mitigation combination.

For LiH (12 qubits before reduction, 4 after active-space reduction), the hardware-efficient ansatz exhibited signs of barren-plateau-like optimization stagnation past 40 parameters, consistent with prior reports in the literature. UCCSD converged more reliably but required roughly 4x the circuit depth. For BeH2, neither ansatz reliably reached chemical accuracy under noise without mitigation; combined mitigation reduced the hardware-efficient ansatz's error from 12.4 mHa to 3.7 mHa, still short of the 1.6 mHa target.

4. Discussion

These results suggest that ansatz selection should be guided by the available circuit depth budget and qubit count rather than by chemical accuracy targets alone. The hardware-efficient ansatz's susceptibility to optimization stagnation as qubit count grows suggests it is best suited to small active spaces on near-term devices, while UCCSD's higher gate count may be prohibitive on hardware with limited coherence time despite its more favourable optimization landscape. The consistent benefit of combining readout-error mitigation with zero-noise extrapolation across all three molecules suggests this pairing as a reasonable default for near-term VQE experiments, though scaling behaviour beyond BeH2-sized systems remains an open question.

5. Conclusion

We benchmarked two VQE ansatz families across three molecular systems under realistic hardware noise and evaluated three error-mitigation strategies. Combined readout-error mitigation

and zero-noise extrapolation consistently improved energy estimates across all tested systems, recovering chemical accuracy for H2 and LiH but not for BeH2. Future work should examine adaptive ansatz construction methods and evaluate these findings on physical hardware rather than simulated noise models.

References

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