Scalable quantum computational chemistry with superconducting qubits

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Quantum chemistry is one of the most promising applications of quantum computing with wide applications in chemistry, drug discovery, material science, etc. Recent theoretical and experimental works have demonstrated the potentiality of solving molecular electronic structures with existing quantum hardware. However, scalable realisations of these algorithms on current quantum devices remain challenging. The state-of-the-art experiments are either restricted to a few qubits or have limited scalability or accuracy. Here, integrating experimental and theoretical advances in more accurate operations and dedicated optimisation of the algorithm, we show an implementation of variational quantum eigensolver with a scalable and optimised multi-reference unitary coupled cluster circuit for H₂, LiH, F₂ from 4 to 12 qubits. Combining error mitigation schemes, we show high-accuracy results of the ground-state energy with around two orders of suppression in errors, and we achieve chemical accuracy for H₂ at all bond distances and LiH at small bond distances. Our work demonstrates a feasible path to a scalable solution to electronic structure calculation, validating key technological features and identifying future challenges for this goal.

I. INTRODUCTION

Quantum computers have great potential to solve classically challenging many-body physics problems, particularly the molecular electronic structure in quantum chemistry [1–3]. Many quantum algorithms [4–8] have been proposed to simulate molecules with deep quantum circuits using fault-tolerant quantum computers, which are yet far beyond the current technology [9]. Meanwhile, recent theoretical and experimental results considered the variational quantum eigensolver (VQE) method [10–12], which relieves the requirement for quantum computing with the assistance of classical optimisation and thus potentially enables the solution of electronic structures using current and near-term quantum devices [2, 3]. Indeed, in the post-quantum supremacy era [13, 14], quantum computational chemistry [2, 3, 15–17] has become one of the promising candidates for realising practical quantum advantages in the near future.

Since the first experimental demonstration of VQE in 2014 [10], a variety of experimental implementations for quantum chemistry problems from H₂ (2 qubits) [10, 18], LiH (4 qubits) [19], BeH₂ (6 qubits) [20] to H₁₂ (12 qubits) [21] and others [22–26] have been reported. However, many of the experiments are either at a small scale or restricted, assuming either nonscalable (hardware efficient) or classically simulable (Hartree-Fock) ansatz. The unitary coupled cluster (UCC) ansatz is believed to be scalable and accurate [27–29]. However, its implementation remains challenging, and its experimental demonstration is still limited to a few qubits [18, 23, 24]. Along with circuit ansatz, we face crucial challenges, including deep circuit depth, large measurement costs, and experimental errors. Any of these factors could significantly affect the accuracy or efficiency of the algorithm and thus restrict the experimental demonstration for quantum chemistry problems.

In this work, we address these challenges with a systematic study of the molecular electronic structure problem. To enable the efficient implementation of the algorithm, we consider a multi-reference initial state, design an efficient circuit by selecting operators from the UCC operator pool, which conserve the molecular symmetry and have dominant contributions to the energy decrease, and compile it into a 2D grid structure with a reduced circuit depth. To optimise the parameters efficiently, we consider stochastic gradient descent with analytical gradients from the parameter shift rule [30] and apply a refined overlapped grouping measurement scheme [31] that speeds up the measurement process. Finally, to suppress
FIG. 1. A diagrammatic scheme for the variational quantum eigensolver on a superconducting quantum processor: device, quantum circuit, measurement, and error mitigation. Mid: The experimental circuit for the 12-qubit $F_2$ VQE experiment over a $2 \times 6$ qubit grid on the “Zuchongzhi 2.0” quantum processor. Mid left: Topology of qubits on the quantum processor. The twelve selected qubits used in the experiments with the encoding of spin up and spin down are coloured. Mid right: Schematic diagram of the VQE process. Top left: Selection of the operators from the UCC operator pool that contribute dominantly to the energy decrease. Top mid: The elementary gate in UCC, which is composed of CNOT gates, single-qubit Pauli rotation gates, and single-qubit Clifford gates. The single-qubit Pauli rotation is decomposed into the $YZY$ gate in our experiment. Top right: An example of the overlapped grouping method for measuring observables, which exploits the qubit-wise compatibility of the observables. Below: Hardware optimisation and error mitigation techniques integrated into the experiments. Distortion correction and dynamical decoupling are first applied to improve the fidelity of the basic operators and suppress dephasing during idle times, respectively. Then readout error mitigation, Clifford circuit fitting, symmetry verification, and connected moment expansion are applied sequentially to calculate the error-mitigated observable expectation values.

We briefly summarise the basic building blocks of the algorithm and refer to Supplementary Information for a detailed discussion. We consider second-quantised molecular Hamiltonians $\hat{H}$ under the Born-Oppenheimer approximation and Jordan-Wigner transformation. We apply variational quantum eigensolver (VQE) to find the ground state of $\hat{H}$. The main idea is to prepare a parametrised quantum state $|\Psi(\theta)\rangle$ by a quantum processor and update the parameters classically. A physically inspired choice for $|\Psi(\theta)\rangle$ is the unitary coupled-cluster (UCC) ansatz $|\Psi(\theta)\rangle = \exp (T(\theta) - T^\dagger(\theta))|\Psi_0\rangle$, which effectively considers excitations and de-excitation above the reference state $|\Psi_0\rangle$ [22–25]. Here $T(\theta)$ is the truncated cluster operator concerning first- and second-order excitations from occupied orbitals to virtual or-
bital. However, direct implementation of UCC on a quantum computer requires CNOT gates scaling as \(O(N(N-\eta)^2\eta^2)\) with system size \(N\) and electron number \(\eta\), which goes beyond the limit of the current technology.

To reduce the gate count, we design the circuit by selecting the operators from the UCC operator pool, which satisfy the symmetry constraint imposed by the selection rule [37]. Moreover, the operators in \(\hat{T}\) have different effects on the ground state, and we thus adopt a classically efficient algorithm to select the qubit operators \(\hat{V}\) that contribute dominantly to the ground state energy decrease [38]. For instance, the total gate count is reduced by two orders of magnitude for \(N=12\). Furthermore, we compile the circuit according to the 2D topology structure of the superconducting processor to reduce the circuit depth. The gate count and circuit depth reduction strategies are scalable and essential for the efficient implementation of UCC ansatz. We illustrate the procedures in Fig. 1.

In VQE, the ground state is approximated by solving \(\min_\theta \langle H \rangle_\theta\) using a classical optimiser of stochastic analytic gradient descent. For the \(k\)-th iteration with parameters \(\theta^k\), we obtain the gradient element \(g_k^j(\theta^k)\) by the parameter shift rule, which requires the measurement of \(\langle H \rangle_{\theta^k}\) with \(\theta^k = \theta^k \pm \pi \Delta^k e_j / 2\) and unit vector \(e_j\) [30]. We stochastically choose the parameters to be optimised to reduce the sample cost for the estimation of gradients. The gradient estimation is unbiased, and has a smaller variance compared with the finite difference method. The parameters are updated by \(\theta^{k+1} = \theta^k + \alpha^k g^k(\theta^k)\) with the learning rate \(\alpha^k\) until convergence. For each \(\langle H \rangle_{\theta^k}\), it generally consists of \(O(N^4)\) terms, whose measurement cost could be prohibitively large in practice. However, as many of the observables have small coefficients and are qubit-wise compatible (hence could be measured simultaneously), we could exploit more efficient measurement schemes to alleviate the measurement cost. Specifically, we apply a refined overlapped grouping measurement scheme [31, 39], which significantly reduces the required measurement count and hence the running time by two orders of magnitude for \(F_2\) compared to importance sampling.

In order to implement the algorithm experimentally and obtain reliable results, we need to optimise the quantum processor and mitigate the experimental errors. We employ various strategies to optimise the gate operations and mitigate different kinds of errors appearing in the circuit and measurement. We apply dynamical decoupling sequences to suppress dephasing errors for idle qubits and introduce a calibrated implementation of basic operations in the circuit to improve the circuit fidelity. We further integrate several error mitigation methods for the remaining errors. For measurement errors, we apply readout error mitigation (REM) to the classical measurement outcomes [32]. For gate errors, we adopt three types of error mitigation methods. Considering the particle number conservation, we apply an effective symmetry verification (SV) of the particle number parity [40]; To mitigate the dominant two-qubit gate errors, we apply Clifford fitting (CF) by learning the noise model from noisy and ideal Clifford circuits [33, 34]; Finally, we apply connected moment expansions (CMX) that effectively implement imaginary time evolution using Hamiltonian moments up to the third order to correct theoretical and experimental imperfections from incapable ansatz and implementation errors [35, 36]. These techniques are essential for accurate experiment implementations of variational quantum algorithms.

![Graphs showing experimental optimisation and implementation of the algorithm.](image-url)
FIG. 3. The VQE simulations for potential energy curves for different molecules. (a-c) Potential energy curves as functions of the bond distance for H\textsubscript{2} (4 qubits), LiH (6 qubits) and F\textsubscript{2} (12 qubits) molecules with various error mitigation strategies. (d-f) Absolute errors are compared to the FCI results. We compare the raw data (yellow squares) with the application of REM and CF (deep blue diamonds), SV (grey-blue triangles) and CMX (red circles). The results marked by green asterisks are energies calculated by classical simulation with the parameters searched in the experiment. The ground state energy with chemical accuracy (blue regime) is calculated theoretically as a reference.

III. RESULTS

The experiment is realised on a 66-qubit superconducting quantum processor “Zuchongzhi 2.0” [14]. We select 12 high-quality qubits arranged in a two-dimensional array shown in Fig. 1. We first optimise the single-qubit gates, CZ gates and readout performance following a series of optimisations (see Supplementary Information). The readout fidelity is 96.3% on average, and the correlated readout error is negligible with the optimisation of readout qubit frequency and suppression of the residual ZZ coupling. The remaining product readout errors are further alleviated by REM. The parallel single-qubit and CZ gate fidelities are 99.90% and 99.19% on average, respectively (see Fig. 2a), characterised by cross-entropy benchmarking (XEB) [13]. The high-fidelity parallel gates are achieved with the advantage of the flip-chip structure and tunable couplers, which suppress the cross-talk significantly. We further optimise the basic operations (consisting of multiple CZ gates and single-qubit operations) in the UCC circuit by correcting the Z pulse distortion on couplers and replacing the amplitude-based Rx(\(\theta\)) gate. As shown in Fig. 2b, the operation fidelity has a notable increase after optimisation and matches the product of the fidelity of the individual quantum gate, indicating its scalability for larger systems.

We apply three error mitigation techniques to further reduce the effects of gate errors: SV, CF, and CMX. For CF, we first run a Clifford analogue circuit of UCC by replacing most of the non-Clifford gates with random Clifford gates. Since Clifford circuits are classically simulable, we can compare the ideal and experimental results, which generally has a linear dependence, as shown in Fig. 2c for the XXYY observable and the 4-qubit H\textsubscript{2} molecule. We refer to Supplementary Information for the implementation and comparison of the other two error mitigation techniques. As shown in Fig. 2d, error mitigation plays a critical role in improving calculation accuracy. In particular, the combination of REM, CF, and SV clearly improves the energy accuracy along the optimisation iteration. CMX further enhances the final energy within the chemical accuracy compared to the ideal ground state energy for the H\textsubscript{2} molecule.

Together with the theoretical and experimental improvements, we now show the calculation of the potential energy curves for H\textsubscript{2} (4 qubits), LiH (6 qubits) and F\textsubscript{2} (12 qubits) molecules. As shown in Fig. 3, we again observe a significant decrease (around two orders) in energy errors with error mitigation for all three molecules. The raw experiment results indicate that the simulation becomes less accurate with an increasing system size, for instance, the error for LiH and F\textsubscript{2} are above 0.1 and 1, respectively. This is because even for the VQE experiment a large number of gates and measurement shots are required, which remains exceptionally challenging for the current hardware. These challenges result in difficulty of demonstration for large molecular systems. In our experiment, we improve the simulation accuracy with device optimisation and error mitigation. In particular, we achieve chemical accuracy for H\textsubscript{2} at all bond distances and LiH at small bond distances. The error increases
for large bond distances for LiH since UCC becomes less accurate in the dissociation regime, which is alleviated by optimised initial state preparation, such as a multi-reference state which is a superposition of the Hartree-Fock state and the dissociated state, see Supplementary Information. Owing to the larger system size and deeper circuit depth, the energy errors for F$_2$ are around $10^{-1}$ to $10^{-2}$, above the chemical accuracy threshold. Nevertheless, if we numerically calculate the energy using the experimentally found parameters, the error could be consistently suppressed below $10^{-2}$. The experimental results indicate that the gate and readout fidelities need to be further improved in order to decrease the error below the chemical accuracy.

With the results of the three molecules, we analyse the resource cost and scalability of VQE in our experiment. As shown in Fig. 4a, our optimisation strategy consistently reduces the gate count and circuit depth of UCC for molecules with different system sizes. The circuit reduction strategy are scalable and crucial for the extension to larger molecules. Comparing the three molecules with an increasing system size in Fig. 4b, we also find that the resource cost (running time and measurement shots) increases almost linearly. Nevertheless, we need to pay more attention to calculation accuracy. The major error sources include readout and gate errors. We analyse their contribution to the energy calculation in Fig. 4c. We find that readout errors dominate for small molecules, while gate errors become more serious when the system size increases. We thus need to systematically improve the readout and gate fidelities to achieve high accuracy for large molecules.

IV. DISCUSSION

In this work, we experimentally implement variational quantum eigensolver with the UCC ansatz for quantum computational chemistry. We show that with dedicated theoretical improvements and experimental optimisations, we can achieve chemical accuracy for H$_2$ at all bond distances and LiH at small bond distances. We observe a significant enhancement of the accuracy to be around two orders with a combination of different quantum error mitigation techniques for the three molecules. We also find that the current hardware is still insufficient for larger molecules, such as F$_2$, mostly owing to non-negligible hardware errors. Our resource analysis indicates the necessity for improved gate and readout operations to achieve chemical accuracy for large molecules.

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