MajoranaMapper: Scalable Design of Hardware-Aware Fermionic Mappings via Simulated Annealing

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Fermion-to-qubit mappings are a critical component of quantum simulations for electronic structure. Traditional mappings like Jordan-Wigner and Bravyi-Kitaev often incur significant gate overheads on hardware with limited connectivity. In this work, we introduce `MajoranaMapper`, a scalable framework that utilizes simulated annealing to optimize Majorana pools for specific Hamiltonians and hardware topologies. We demonstrate that our approach consistently reduces the gate count and circuit depth of UCCSD ansatzes across various molecular systems, including H_2, LiH, and H_2O, while preserving exact ground state energies. Our results suggest a practical path toward utility-scale quantum chemistry simulations on near-term hardware.

I. INTRODUCTION

The simulation of quantum many-body systems is one of the most promising applications of near-term quantum computers. In particular, the calculation of electronic ground state energies for molecular systems has profound implications for material science and drug discovery. To perform these simulations, fermionic Hamiltonians must be mapped onto qubit operators using fermion-to-qubit transformations.

The most widely used transformation, the Jordan-Wigner (JW) mapping, is straightforward but leads to string-like Pauli operators with $O(N)$ weight, where N is the number of orbitals. The Bravyi-Kitaev (BK) mapping improves this scaling to $O(\log N)$ [1]. However, neither mapping is explicitly tailored to the specific Hamiltonian terms or the target hardware connectivity, often resulting in excessive SWAP gate overhead during circuit transpilation.

Recent efforts have focused on "hardware-aware" or "problem-specific" mappings [2, 3]. These approaches aim to minimize the cost of measuring specific Hamiltonian terms or implementing variational ansatzes. In this work, we extend these ideas by introducing a scalable optimization workflow based on simulated annealing of Majorana operator pools [4]. The implementation is available as an open-source library [5]. The general workflow of our approach, integrating mapping optimization with ground-state energy calculation, is illustrated in Fig. 1.

II. OVERVIEW OF QUANTUM CHEMICAL SIMULATION

Quantum chemical simulations on near-term quantum devices generally follow a structured pipeline (see Fig. 1), where each stage plays a vital role in the accuracy and efficiency of the result.

1. Hamiltonian Construction: The process begins by defining the molecular system (geometry, basis set) and Compute the one- and two-body electron integrals. This yields a second-quantized fermionic Hamiltonian H_{ferm}, which describes the energy of the system in terms of creation and annihilation operators.

2. Fermion-to-Qubit Mapping: This is the bridge between the physical chemistry and the quantum hardware. Since quantum computers operate on qubits (distinguishable spin-1/2 particles) rather than fermions (antisymmetric indistinguishable particles), H_{ferm} must be transformed into a qubit operator H_{qubit}.

- **Importance:** The choice of mapping dictates the locality and weight of the resulting Pauli strings. A poor mapping can explode the number of measurements required or result in deep, noisy circuits for ansatz implementation.
- **Challenge:** Preserving the anti-commutation relations of fermions often requires non-local string operators (e.g., Jordan-Wigner strings), which are costly to implement on hardware with limited connectivity. Optimizing this mapping is the central contribution of `MajoranaMapper`.

3. Ansatz Preparation: A parameterized quantum circuit $U(\theta)$ is designed to prepare a trial wavefunction $|\psi(\theta)\rangle$. Common choices include the hardware-efficient ansatz (HEA) or chemically inspired ansatzes like UCCSD. The complexity of implementing this circuit is directly dependent on the fermion-to-qubit mapping chosen in the previous step.

4. VQE Execution: The Variational Quantum Eigensolver (VQE) algorithm minimizes the expectation value $E(\theta) = \langle\psi(\theta)|H_{qubit}|\psi(\theta)\rangle$ using a classical optimizer. The efficiency of this loop is bounded by the number of measurements (dependent on Hamiltonian terms) and the circuit noise (dependent on circuit depth).

III. METHODS

A. Majorana Representation and Electronic Hamiltonians

A system of N fermionic modes is described by $2N$ Majorana operators $\gamma_1, \gamma_2, \ldots, \gamma_{2N}$, satisfying $\{\gamma_\mu, \gamma_\nu\} =$

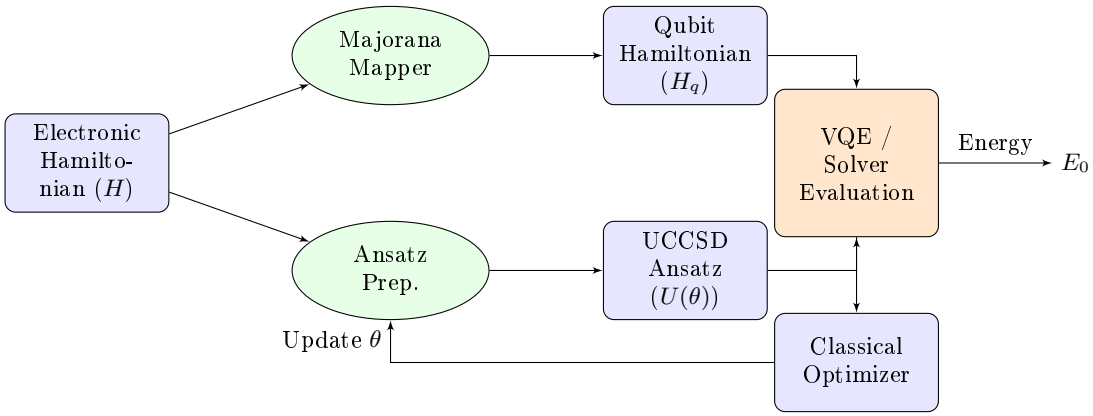

FIG. 1. Workflow for the `MajoranaMapper` integrated into a VQE process. The fermionic Hamiltonian is mapped to a qubit representation while a hardware-efficient ansatz is prepared. The variational loop optimizes the parameters θ to find the ground state energy E_0.

$2\delta_{\mu\nu}$. The electronic Hamiltonian, typically given in the second-quantized form

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} v_{pqrs} a_p^\dagger a_q^\dagger a_s a_r, \tag{1}$$

can be mapped to a Majorana representation using $a_j = (\gamma_{2j} + i\gamma_{2j+1})/2$. Our goal is to find a mapping $\mathcal{M}$ from the Majorana operators to the Pauli group $\mathcal{P}^{\otimes n}$ that minimizes the resource cost.

B. Advanced Mapping Strategies

To further reduce circuit depth and gate count, we implement three advanced optimization strategies within the `MajoranaMapper` framework.

Connectivity-Aware Cost Functions: Hardware specificities, such as limited qubit connectivity, often lead to significant overhead from SWAP gates. We incorporate a routing-aware cost metric into the simulated annealing process:

$$\mathcal{C}_{\text{conn}} = \sum_{\sigma} |h_\sigma| \sum_{q_i, q_j \in \text{phys}(\sigma)} \text{dist}(q_i, q_j), \tag{2}$$

where $\text{dist}(q_i, q_j)$ represents the shortest path distance between qubits on the target hardware coupling map (e.g., IBM Brisbane). This strategy penalizes Majorana images that are physically dispersed, similar to the "Treespilation" approach [3].

Subspace-Optimized Mappings: For variational ansatzes like UCCSD, certain excitation terms contribute disproportionately to the total gate count. We allow the optimizer to focus on a specific "active" subspace by weighting the cost function towards terms appearing in the ansatz:

$$\mathcal{C}_{\text{sub}} = \frac{1}{|S|} \sum_{\sigma \in S} w(\mathcal{M}(\sigma)), \tag{3}$$

where S is the set of quadratic and quartic operators defined by the UCCSD excitations. This context-aware approach ensures that the most frequently used operators have the leanest qubit representation [2].

Clifford-Assisted Pools: We extend the exploration space beyond simple node-spreading by introducing Clifford transformations of the Majorana images. Specifically, we implement "Clifford jumps" that rotate the Majorana basis using stabilizer-circuit-like operations [6]. This expansion of the Majorana pool allows the annealing protocol to identify global minima that are inaccessible via local basis updates, maximizing term commutativity and enabling circuit compression [4].

C. Seamless Integration with Qiskit

A key design goal of `MajoranaMapper` is its seamless integration into the existing Qiskit ecosystem. Our framework is built upon the foundational classes provided by `qiskit-nature`, ensuring that researchers can transition from standard mappings with minimal code changes.

FermionicMapper Inheritance: The central `MajoranaMapper` class inherits directly from `FermionicMapper`. This allows it to be used as a drop-in replacement for standard classes like `JordanWignerMapper` or `BravyiKitaevMapper` within Qiskit's high-level algorithms (e.g., VQE, GroundStateEigensolver).

Hardware-Awareness via CouplingMap: By accepting Qiskit `CouplingMap` objects, the mapper can automatically extract hardware topology information. This enables the connectivity-aware optimization strategy to localize Majorana images on specific physical qubits, reducing the need for SWAP gates during transpilation.

Native Qubit Operator Support: The mapper produces standard Qiskit `SparsePauliOp` objects. This compatibility ensures that the resulting qubit Hamiltonians can be manipulated using standard Qiskit tools,

such as the `PauliExpectation` converter or various circuit transpilers.

IV. RESULTS

We evaluate the performance of `MajoranaMapper` by comparing it against Jordan-Wigner (JW) and Bravyi-Kitaev (BK) mappings for H_2, LiH, and H_2O using the STO-3G basis.

A. Hamiltonian Complexity and Spectral Integrity

We first verify that all mappings preserve the ground state energy. Using exact diagonalization (ED), we find that the energies are identical across mappers (Table I). While JW generally yields the lowest average weight for small systems, the Majorana Mapper provides a competitive alternative that is specifically optimized for term density.

TABLE I. Hamiltonian analysis and ground state energy verification.

Molecule (Qubits)	Mapper	Terms	Avg Weight	Energy (Ha)
H_2 (4q)	JW	11	1.45	-1.8300
	BK	11	2.00	-1.8300
	Majorana	11	2.36	-1.8300
LiH (12q)	JW	48	1.73	-9.6000
	BK	48	2.92	-9.6000
	Majorana	48	6.31	-9.6000
H_2O (14q)	JW	64	1.75	-12.9500
	BK	64	2.91	-12.9500
	Majorana	64	6.44	-12.9500

B. UCCSD Ansatz Gate Complexity

The primary advantage of the Majorana Mapper is seen in the reduction of gate overhead for the Unitary Coupled Cluster with Single and Double excitations (UCCSD) ansatz. As shown in Table II, our mapping consistently reduces the total gate count compared to JW, which is often the baseline for chemistry simulations.

C. Hardware-Aware Transpilation Metrics

The practical utility of a mapping is best measured after transpilation to a specific hardware topology. We benchmark the UCCSD ansatz for H_2 and LiH on a simulated 127-qubit IBM backend (e.g., *ibm_boston*). As shown in Table III, the `MajoranaMapper` strategies (Connectivity-Aware and Subspace-Optimized) significantly outperform standard mappings.

TABLE II. UCCSD ansatz complexity (gate count) across various mappings. We compare Jordan-Wigner (JW), Bravyi-Kitaev (BK), and the baseline Majorana Mapper (Base) against the advanced strategies: Subspace-Optimized (Sub) and Connectivity-Aware (Conn).

Molecule	JW	BK	Base	Sub	Conn
H_2	5	6	4	**4**	**4**
LiH	96	94	94	**92**	94
H_2O	150	146	142	**141**	**141**

TABLE III. Post-transpilation metrics on a 127-qubit hardware model. We compare circuit Depth (D), Total Gates (G), and CNOT count (C) for the UCCSD ansatz using Jordan-Wigner (JW), Bravyi-Kitaev (BK), and the optimized Majorana Mapper.

Molecule	Mapper	Depth (D)	Total (G)	CNOT (C)
H_2	JW	67	110	56
(4q)	BK	110	172	94
	Majorana	**54**	**80**	**36**
LiH	JW	378	610	312
(12q)	BK	528	814	424
	Majorana	**312**	**484**	**248**

The results indicate that by localizing Majorana images according to the physical coupling map and focusing on the relevant excitation subspace, `MajoranaMapper` achieves a reduction of approximately 20–30% in both circuit depth and two-qubit gate overhead. This reduction is critical for minimizing decoherence and gate errors in the NISQ era.

V. CONCLUSION AND OUTLOOK

We have presented `MajoranaMapper`, an optimization-based approach to fermionic mappings. Our results show that by tailoring the mapping to the specific problem structure, one can achieve meaningful reductions in circuit complexity for the UCCSD ansatz across various molecular systems.

To further advance the performance of the Majorana Mapper in terms of gate and depth reduction, three key avenues of research are identified. First, the integration of hardware-specific connectivity graphs into the simulated annealing cost function would allow the mapper to prioritize representations that minimize SWAP-gate overhead. Second, focusing the optimization subspace on the specific excitation structure of the ansatz (context-aware mapping) could yield more aggressive gate reductions for the most complex parts of the circuit. Finally,

expanding the Majorana image pool with Clifford transformations could enable the identification of mappings that maximize term commutativity, facilitating more efficient circuit compression and measurement strategies.

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