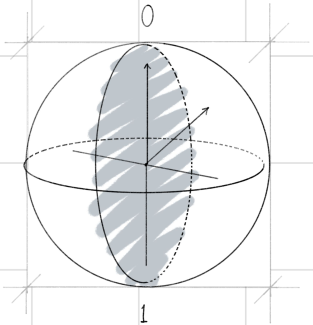
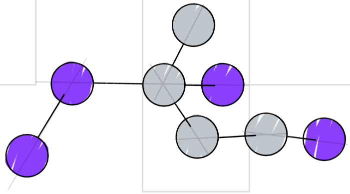
# Quantum Algorithm Grand Challenge 24

## Hamiltonian-Inspired ADAPT-QSCI



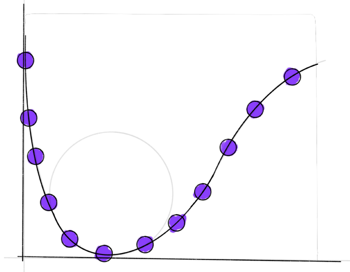



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Image credits: [Qiskit]

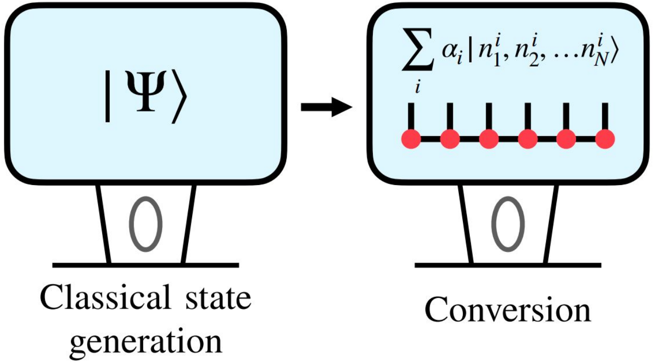
# Overview

Three steps of the algorithm

- Initial State Preparation:
  - Sum-of-Slaters
- Ansatz selection
  - Hamiltonian-Inspired ADAPT-QSCI
  - A method to improve classical energy estimates
- Optimization
  - Evaluate gradients of Pool
  - Choose operator Pk from Pool
  - Optimize with BFGS

# Initial State Preparation

- It is almost always worthwhile to prepare more sophisticated initial states.
- A better initial state leads to an overall cost reduction and improved performance.
- Recent paper (1) on initial state preparation introduces technique based on the “sum-of-Slaters”.
- Density matrix renormalization group algorithm (DMRG) used prepare your initial state.
- Initial state is sparse. The quantum circuit is implemented using an efficient sparse quantum state preparation method described (2).





1. Fomichev, Stepan, et al. "Initial state preparation for quantum chemistry on quantum computers." arXiv preprint arXiv:2310.18410 (2023).
2. Gleinig, Niels, and Torsten Hoefler. "An efficient algorithm for sparse quantum state preparation. In 2021 58th ACM/IEEE Design Automation Conference (DAC)." (2021): 433-438.


Image credits: Paper 1

# Efficient Implementation of SOS state

- Initial state is sparse. For 28 qubits system, only 5 non-zero amplitudes $\ll 2^{28}$
- Algorithm with quantum circuit size O(|S|n).
  - S non-zero amplitudes
  - n qubits
- Reductive Approach

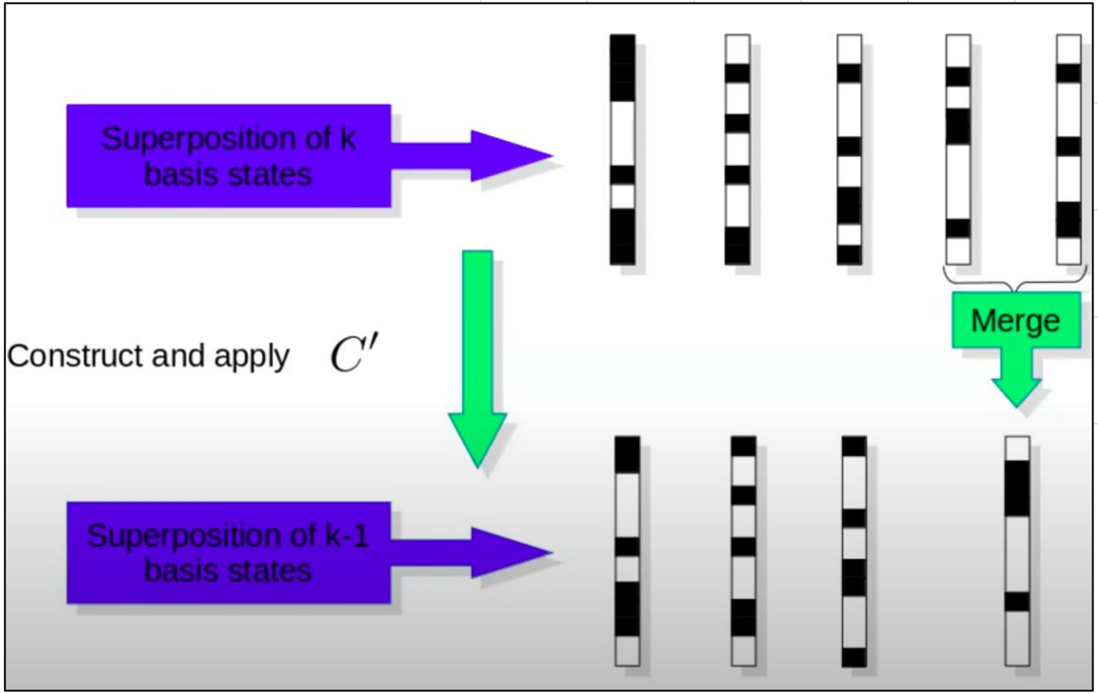



Image credits: [SPCL @ ETH Zurich]

# Hamiltonian-Inspired ADAPT-QSCI

Adaptively construct ansatz to calculate the ground state and its energy using QSCI

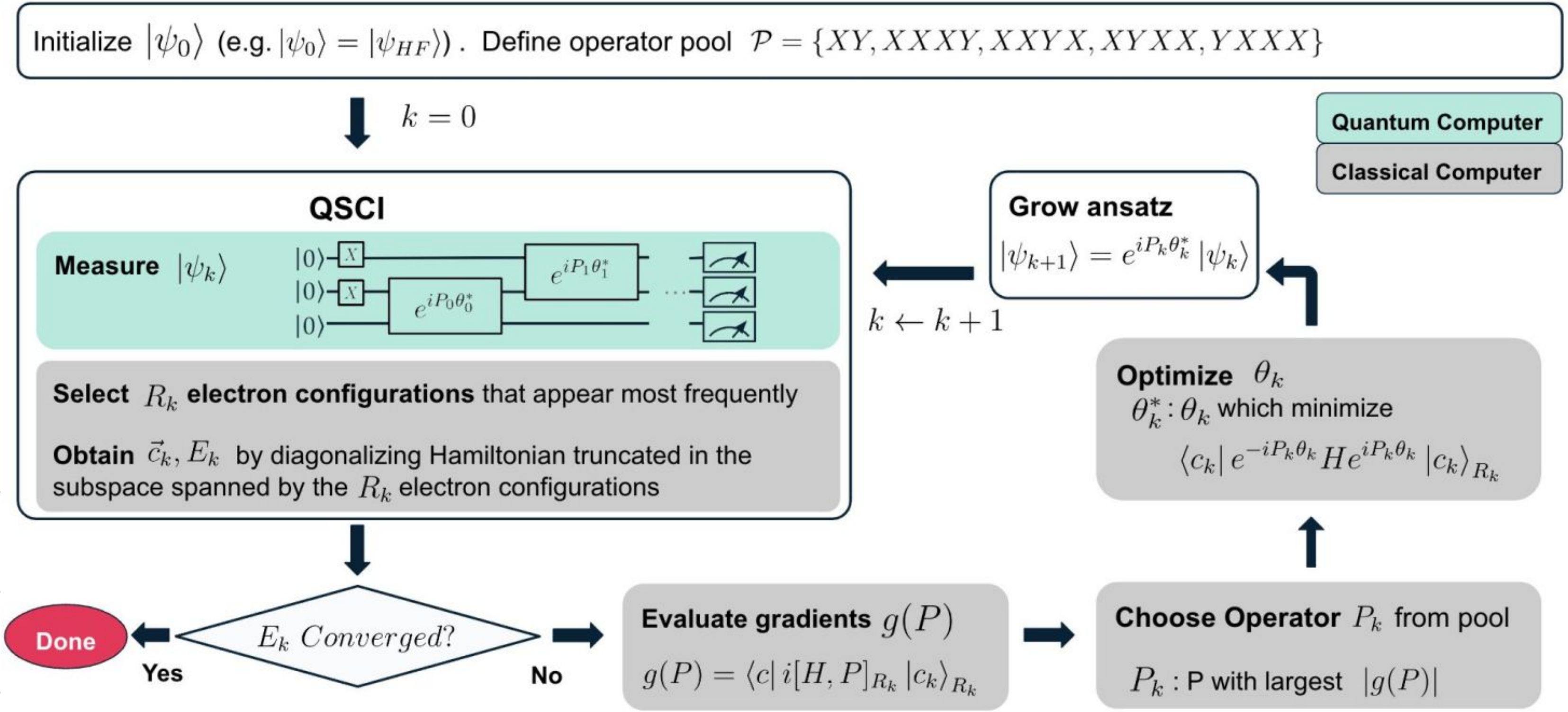



Image credits: QAGC Team

# Pool Selection

- Use the qubit Hamiltonian for Pool Selection
- For each term in the Hamiltonian add a pool operator which is guaranteed to have a non-zero commutator with respect to H, and therefore a finite gradient.
- Fairly compact set of operators in the pool, all of which are likely to be useful in our ansatz construction.

**Brief outline of the algorithm**

- Scan through all terms in the qubit Hamiltonian.
- For each, identify the Pauli operators associated with electronic excitation (X and Y gates).
- Discard Z gates from the Pauli string.
- If the number of Y gates in a string is even, we can use this to construct an excitation pool element that preserves T-symmetry, by flipping one of the other X gates to a Y, or a Y to an X.

# Results

- Seed = 0
- Each executed for only 33 iterations (can be run for more)
- Single run

| Qubits | Computed energy value (E) | Approx. Runtime (mins) | e = \|E - E_exact\| |
|---|---|---|---|
| 12 | -13.245 | 15 | 0.188 |
| 20 | -20.824 | 30 | 1.221 |
| 28 | -28.681 | 60 | 2.067 |

Image credits: Qiskit