Quantum Chemistry on Fault-tolerant Quantum Computers: Unitary Downfolding and Spectral-Range Reduction for Faster QPE

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Project Summary

Quantum Phase Estimation (QPE) is a flagship algorithm for fault-tolerant quantum computers and offers a path to highly accurate molecular energies. The challenge is cost: the quantum runtime can be dominated by Hamiltonian simulation, which depends strongly on the Hamiltonian's spectral range and on how efficiently it can be represented as a sum of simple unitary operations. This project investigates practical "Hamiltonian engineering" ideas—downfolding and spectral compression—to make QPE-style algorithms significantly cheaper for quantum chemistry.

Project Description

The central idea is to reduce the effective energy scale of the molecular Hamiltonian without changing the chemically relevant low-energy physics. We will study unitary downfolding methods that partition orbitals into an active (internal) space and an external space, then apply a sequence of analytically defined unitary transformations that progressively decouple (and effectively integrate out) the external degrees of freedom. The output is an effective Hamiltonian acting only on the active space, but still capturing important correlation effects from the full system.

For fault-tolerant simulation approaches based on qubitization / linear-combination-of-unitaries (LCU), the cost is closely tied to quantities like the LCU "1-norm" and the Hamiltonian's spectral range. We will explore how downfolding plus symmetry-preserving spectral shifts can compress these quantities, leading directly to reduced gate counts for QPE (and related algorithms).

What you'll do

- Read and discuss key background papers on QPE, Hamiltonian simulation, and unitary downfolding.
- Implement small-scale prototypes in Python and test spectral-range / cost reductions on toy models and small molecules (e.g., H_2, LiH, H_2O in minimal bases).
- Compare different choices of active spaces and compression strategies; summarize results in a short report and final presentation.

Requirements

- Comfort with Python and linear algebra; curiosity and persistence with open-ended problems.

- Basic quantum mechanics is required.
- Helpful (but not required): familiarity with quantum chemistry (second quantization), or introductory quantum computing.

Suitable for

Chemistry, Physics, Mathematics, Computer Science, Electrical/Computer Engineering, or related programs.

Reference

S. Patel, A. S. Brahmachari, J. T. Cantin, L. Wang, and A. F. Izmaylov, "Global Minimization of Electronic Hamiltonian 1-Norm via Linear Programming in the Block Invariant Symmetry Shift (BLISS) Method," J. Chem. Theory Comput. 21, 703–713 (2025) (arXiv:2409.18277).

Quantum Chemistry on Near-term Quantum Computers:
Symmetry-based Circuit Reduction and Efficient Measurements (Q-SENSE Extensions)

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Project Summary

Molecular electronic structure problems are among the most promising applications of quantum computing, but today's noisy (NISQ) hardware can only run shallow circuits and has limited measurement bandwidth. This project develops and benchmarks algorithmic ideas that directly target the two biggest practical bottlenecks in near-term quantum chemistry: (1) reducing circuit depth and (2) reducing the number of measurements needed to estimate energies and properties.

Project Description

We will build on Quantum SENiority-based Subspace Expansion (Q-SENSE), a hybrid quantum-classical framework that replaces deep variational circuits with a small, symmetry-structured subspace calculation: we prepare and relate short-circuit basis states on the quantum device, measure Hamiltonian matrix elements, and solve the resulting eigenvalue problem classically. The research direction for this project is to extend Q-SENSE using different local symmetries (beyond seniority) to construct orthogonal basis states, suppress unnecessary couplings, and further reduce circuit complexity. In parallel, we will explore symmetry-aware measurement strategies (e.g., commuting-grouping and overlap-based estimators) to cut the total measurement cost.

What you'll do

- Read and discuss key background papers (Q-SENSE and related subspace / VQE methods).
- Implement small-scale prototypes in Python and benchmark resource metrics (two-qubit gate depth, number of circuits, and shot counts) on toy models and small molecules (e.g., H2, LiH in minimal bases).
- Compare different symmetry choices and measurement strategies; summarize results in a short report and final presentation.

Requirements

- Comfort with Python and linear algebra; curiosity and persistence with open-ended problems.
- Basic quantum mechanics is required.
- Helpful (but not required): familiarity with quantum circuits / Pauli operators, Qiskit or PennyLane, or introductory quantum chemistry.

Suitable for

Chemistry, Physics, Mathematics, Computer Science, Electrical/Computer Engineering, or related programs.

Reference

S. Patel, P. Jayakumar, T. Zeng, and A. F. Izmaylov, “Quantum Seniority-based Subspace Expansion: Linear Combinations of Short-Circuit Unitary Transformations for Efficient Quantum Measurements,” arXiv:2509.01061 (2025).