Simulating Complex Molecular Interactions Using Quantum Harmonic Oscillators

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ABSTRACT

- Hybrid quantum computers combining **discrete variables (qubits)** and **continuous variables (qumodes)** provide a promising framework for simulating molecular dynamics beyond classical and purely qubit-based approaches
- The **Hamiltonian** of a system represents its total energy and governs its evolution
- Molecular dynamics can be approximated by parameterized quantum gate sequences acting on **quantum harmonic oscillators (continuous variables)**
- Parameter optimization becomes increasingly computationally expensive and unstable at longer evolution times
- We benchmark optimization strategies using the **Morse Hamiltonian** to improve parameter fitting accuracy, convergence stability, and runtime performance

BACKGROUND

Qubits and qumodes are basic units of quantum information. Qubits can be in the 0 or 1 state (physically realized by the bottom 2 levels of an anharmonic oscillator, seen in figure 2), or a superposition of those states. Qumodes can be in any of an infinite number of different states or any superposition of those states (physically realized by the energy levels of harmonic oscillators).

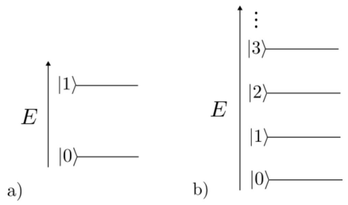

Figure 1: Distinct states of a qubit (a) compared with the infinitely distinguishable states of an oscillator (b)[1].

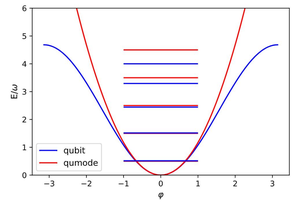

Figure 2: First five energy levels of a transmon qubit (blue) and an oscillator (red)[1].

The Morse Potential is a specific interatomic interaction model that describes the potential energy of a diatomic molecule. This model has a limited number of defined energy states, seen in figure 3.

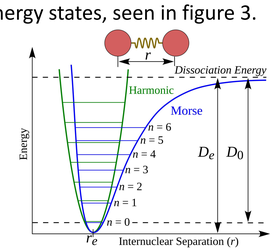

Figure 3: Limited energy levels defined by the Morse Potential Compared to the infinite levels of an Oscillator[2].

$$\hat{H} = \frac{1}{2\mu}\hat{p}^2 + D(1 - e^{-\beta(\hat{q}-q_0)})^2$$

Equation 1: Full equation for the Morse Hamiltonian. Where μ is the diatomic mass, $\hat{p}$ is the momentum operator, D is the well depth (seen in figure 3), β controls the width of the potential (seen in figure 3), $\hat{q}$ is the distance between atoms, and q_0 is the equilibrium length of the bond.

Approximating time evolution under molecular Hamiltonians requires fitting parameterized quantum gate sequences across increasing evolution times. As evolution time grows, the optimization landscape becomes complex, leading to poor convergence, sensitivity to initialization, and rapidly increasing computational cost. These challenges motivate the development of strategies that improve optimization stability and scalability rather than relying on brute-force parameter fitting.

OBJECTIVE

Develop and evaluate a robust optimization strategy for fitting parameterized hybrid quantum gate sequences to the time evolution of the Morse Hamiltonian across increasing evolution times.

METHODS

Time evolution was evaluated over times ranging from 0.5 to 3.0 seconds in increments of 0.25 seconds (0.5, 0.75, …, 2.75, 3.0). For each evolution time, two optimization approaches were compared.

First, a brute-force optimization was performed independently at each evolution time, starting from the same initial parameter values. The resulting infidelity and optimization runtime were recorded.

Second, a parameter propagation strategy was employed. Starting at an evolution time of 0.5 seconds, parameters were optimized sequentially at each 0.25-second increment, using the optimal parameters from the previous time step as the initial parameters for the next time step. This process was repeated until the target evolution time was reached. To limit unnecessary computation, optimization at each step was terminated once the infidelity dropped below 0.1%, as further runtime yielded minimal improvement.

Multiple classical optimizers were benchmarked, and BFGS was selected based on its superior convergence performance. The Hilbert space dimension (75) and gate depth (14) were chosen to be sufficiently large to accurately capture the system dynamics while maintaining stable performance across all evolution times tested.

RESULTS

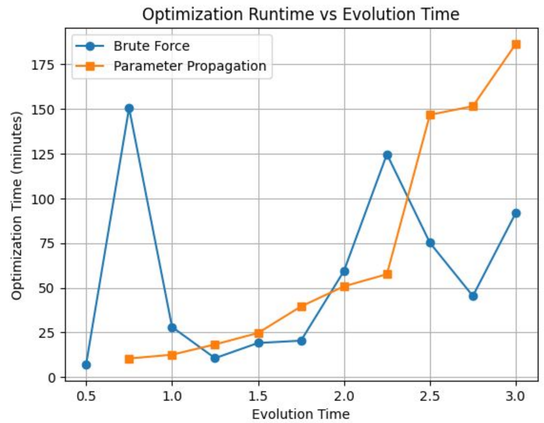

Figure 4: Optimization runtime comparison between brute-force optimization and the parameter propagation strategy for different evolution times. Less is better.

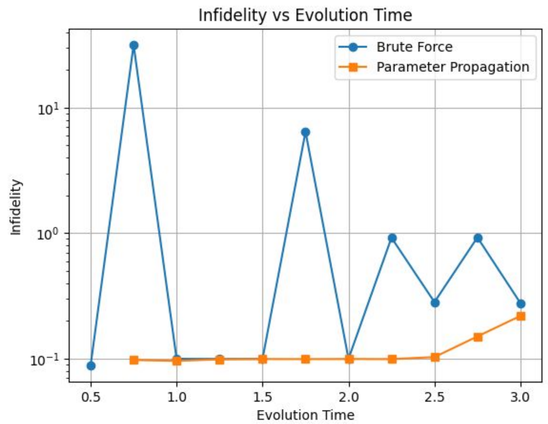

Figure 5: Infidelity comparison between brute-force optimization and the parameter propagation strategy for different evolution times. The lower the infidelity, the closer the simulation is to the true evolution (less is better).

DISCUSSION

The results show no conclusive overall improvement in optimization runtime when using the parameter propagation strategy compared to brute-force optimization. However, parameter propagation exhibits more consistent and predictable runtime behavior across evolution times.

In contrast, brute-force optimization leads to significant instability in infidelity, with frequent convergence failures at scattered evolution times. These failures manifest as abrupt increases in infidelity and unreliable optimization outcomes. The parameter propagation method produces stable and smoothly varying infidelity across increasing evolution times, maintaining high accuracy where brute-force approaches fail.

Although achieving infidelity below 0.1% becomes increasingly difficult at larger evolution times, parameter propagation continues to converge to physically reasonable solutions.

LIMITATIONS & FUTURE DEVELOPMENT

Limitations

- Simulations were performed with gate depths and Hilbert space dimensions sufficient to capture system behavior, but the choice of time-step interval (0.25 s) may not be optimal for all parameter regimes. Preliminary testing showed 0.1 s or 0.5 s intervals can perform worse under the tested conditions, though different combinations of depth, dimension, or circuit parameters may benefit from alternative intervals.
- Simulations were run on a personal laptop, with only VS Code and the simulation active. While sufficient for these proof-of-concept studies, larger systems or longer evolution times may require more powerful computational resources for practical performance and stability testing.
- Current simulations do not include noise, so the results reflect idealized performance of parameter propagation versus brute-force optimization.

Future Directions

- Introduce engineered noise (e.g., amplitude damping, dephasing, leakage) in simulations to study its effect on hybrid quantum gate behavior.
- Use data from noisy simulations to develop a robust benchmarking protocol for hybrid quantum gates under realistic conditions.
- Conduct in-depth studies to determine optimal evolution time intervals, gate depth, and Hilbert space dimensions for different systems.
- Extend simulations to larger Hilbert spaces and more complex molecular models, leveraging high-performance computing resources to evaluate the scalability and robustness of parameter propagation strategies.

REFERENCES & ACKNOWLEDGEMENTS

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