Master Thesis Project in Quantum Information Science and Technology

Parametric Matrix Models for Trotterized Quantum Dynamics

Duration: 1 year

Introduction

Simulating quantum dynamics on quantum computers typically relies on Trotter or Suzuki–Trotter decompositions of the time-evolution operator $U(t) = e^{-iHt}$. While higher-order decompositions reduce the Trotter error, they also increase the circuit depth and thereby make real-device execution more demanding.

The recently introduced *Parametric Matrix Models* (PMMs) provide a new machine-learning architecture whose structure mirrors the matrix equations of physical systems. PMMs can emulate eigenvalues, observables, and even unitary evolution, and show excellent extrapolation properties. In particular, PMMs have been shown to reproduce "zero-error" Trotter extrapolations from data taken at moderate time steps.

This thesis will explore PMMs as a framework for learning effective Hamiltonians corresponding to different Trotter expansions. The goal is to test whether PMMs can systematically reduce Trotter errors, learn Trotterized unitaries, and predict ideal time evolution from noisy quantum hardware. The project will involve both classical simulations and experiments on real quantum computers (IBM Quantum, AWS Braket, or Azure Quantum).

Project Outline

1. **Literature Review and Theory**
   - Review Trotter and Suzuki–Trotter expansions.
   - Study PMMs as introduced in Cook *et al.*, Nature Comm. (2025).
   - Understand eigenvalue-based and unitary-based PMM formulations.
2. **PMMs for Trotter Expansion Learning**

- Implement affine eigenvalue PMMs and affine observable PMMs.
- Construct PMMs that mimic the product structure of Trotterized unitaries.
- Train PMMs on simulated quantum data for various Hamiltonians:
  - Transverse-field Ising model
  - Heisenberg and XXZ chains
  - Fermi-Hubbard model (2–4 qubits)
  - Lipkin–Meshkov–Glick model

3. Benchmarking and Model Comparison

- Compare PMM predictions to:
  - Exact classical simulation
  - Standard polynomial extrapolations of Trotter error
  - Variational quantum algorithms (VQE, Krylov, etc.)
- Evaluate performance across system size, entanglement, Trotter step size, and Hamiltonian complexity.

4. Real-Device Quantum Computing Experiments

- Execute Trotterized unitaries for chosen Hamiltonians on real quantum hardware.
- Collect data at a range of Trotter step sizes dt.
- Train PMMs on real-device output data.
- Evaluate if PMMs can:
  - Extrapolate to the zero-step limit $dt \to 0$,
  - Learn effective Hamiltonians $H_{\text{eff}}(dt)$,
  - Compensate for hardware noise.

5. Extensions and Optional Topics

- PMMs for error mitigation (noise-adapted effective Hamiltonians).
- PMMs as surrogates for quantum simulation (hybrid classical–quantum workflows).
- Study analytic continuation properties and exceptional points.

Milestones

1. **Month 1–2:** Literature review, PMM theory, Trotter theory, Qiskit setup.
2. **Month 3–4:** Implement PMM codebase (Hermitian + unitary PMMs).
3. **Month 5:** Test PMMs on simple 1–2 qubit Hamiltonians.
4. **Month 6–7:** Large-scale simulations of Ising, XXZ, and LMG models.
5. **Month 8:** Run experiments on IBM Quantum or AWS Braket.
6. **Month 9:** Combine real data + PMMs and perform Trotter extrapolation.
7. **Month 10:** Benchmark against VQE, polynomial fits, and exact data.
8. **Month 11:** Write thesis, finalize figures, summarize results.
9. **Month 12:** Complete thesis, prepare presentation.

Expected Outcomes

- A systematic evaluation of PMMs as Trotter-emulation tools.
- A software implementation (Python/Qiskit + PyTorch/Numpy).
- A benchmark suite comparing PMMs to conventional extrapolation methods.
- Demonstrations of PMM-based extrapolation using real quantum hardware.