Master Thesis Project in Quantum Information Science and Technology

Parametric Matrix Models for Trotterized Unitary Coupled Cluster Dynamics of the Pairing Hamiltonian

Duration: One Year (60 ECTS)

1. Introduction

Quantum computing offers new paradigms for solving strongly correlated quantum many-body problems in nuclear physics, quantum chemistry, and condensed matter systems. Among the most prominent variational quantum algorithms is the *unitary coupled cluster* (UCC) approach, where a parametrized unitary ansatz

$$U(\boldsymbol{\theta}) = e^{T(\boldsymbol{\theta}) - T^{\dagger}(\boldsymbol{\theta})}$$

is used to prepare approximate ground states of interacting Hamiltonians, such as the pairing Hamiltonian relevant for superconductivity and nuclear pairing correlations.

On a digital quantum computer, UCC operators must be decomposed into sequences of elementary quantum gates using Trotter–Suzuki factorizations. The finite Trotter step size Δt (or, more generally, the finite number of Trotter steps) introduces systematic errors. Reducing Δt improves accuracy but increases the number of gates, which is problematic for near-term noisy intermediate-scale quantum (NISQ) devices.

Recently, Cook *et al.* introduced *Parametric Matrix Models* (PMMs) as a physics-inspired machine learning framework based on parametrized Hermitian or unitary matrices and their eigenvalues/eigenvectors. PMMs are universal function approximators that work directly with matrix equations, and they have been used to perform *zero-error Trotter step extrapolation* in quantum simulations by learning the dependence of observables on the Trotter step size and extrapolating to the continuum limit.

This master thesis aims at combining the PMM framework with Trotterized UCC simulations of a pairing Hamiltonian (reduced BCS Hamiltonian) relevant for nuclear structure and superconductivity. The project will focus on classical simulations of the quantum circuits (e.g. in Qiskit or similar libraries), generation of Trotterized data, and the construction and training of PMMs to extrapolate observables and energies to the $\Delta t \to 0$ limit in an efficient and interpretable way.

2. Scientific Background and Motivation

The pairing Hamiltonian is a minimal yet non-trivial model for fermionic superfluidity and nuclear pairing:

$$H = \sum_{p} \varepsilon_p N_p - G \sum_{p,q} P_p^{\dagger} P_q,$$

where N_p are number operators, $P_p^{\dagger}$ and P_p are pair creation and annihilation operators, ε_p are single-particle energies, and G is the pairing strength. This Hamiltonian exhibits strong correlations and can be mapped to a spin representation suitable for quantum simulation.

The UCC ansatz for the pairing Hamiltonian is constructed from physically motivated excitation operators that create and annihilate pairs, and the corresponding unitary transformation is implemented on a quantum device via Trotter factorizations. For a time-independent effective Hamiltonian or UCC generator K, one typically uses approximations of the form

$$e^{-iK\Delta t} \approx \prod_j e^{-iK_j\Delta t},$$

where $K = \sum_j K_j$ and the K_j are simpler terms whose exponentials can be directly decomposed into quantum gates. Repeating this product n times approximates a longer evolution or a more accurate UCC operator, but also increases circuit depth and noise.

The key challenges are:

- Quantifying and mitigating Trotter errors in realistic UCC circuits.
- Extrapolating observables (e.g. ground-state energies, pair occupation numbers) to the zero Trotter-step limit using data obtained at relatively large Δt that are feasible on NISQ devices.
- Designing extrapolation schemes that respect the underlying analytic structure of the quantum evolution and that can be efficiently trained from limited data.

PMMs provide a natural framework for this problem. By learning an effective Hermitian matrix model whose eigenvalues and eigenvectors reproduce the dependence of observables on Δt and the UCC parameters, one can perform robust extrapolations and gain additional insight into the analytic structure of the Trotterized dynamics.

3. Objectives

The overall goal of this thesis is to develop and test a parametric matrix model for Trotterized UCC simulations of the pairing Hamiltonian on quantum computers. The work combines quantum many-body theory, quantum computing, and physics-inspired machine learning.

Objective 1: Theory and Literature Review

- Review the theory of the pairing Hamiltonian (reduced BCS model) and its applications in nuclear physics and superconductivity.
- Study the unitary coupled cluster method and its use in quantum algorithms (UCCSD and pairing-specific UCC variants).
- Understand Trotter–Suzuki expansions and their role in implementing UCC unitaries on quantum hardware.
- Study the theory of Parametric Matrix Models as introduced by Cook *et al.*, including:
  - affine Hermitian PMMs and unitary PMMs,

- eigenvalue-based and observable-based PMM architectures,
- the example of zero-error Trotter step extrapolation presented in the article.

Objective 2: Classical Simulation of the Pairing Hamiltonian and UCC Circuits

- Implement the pairing Hamiltonian in a suitable basis (e.g. spin representation via Jordan–Wigner or Bravyi–Kitaev transformation).
- Construct classical simulations of UCC-type quantum circuits for small systems (few pairs and levels) using a quantum computing framework (e.g. Qiskit).
- Implement Trotterized approximations to the UCC operator and generate data for energies and selected observables as functions of:
  - Trotter step size Δt,
  - number of Trotter steps,
  - pairing strength G and single-particle spacing,
  - UCC parameters (e.g. amplitudes).

Objective 3: Design and Implementation of Parametric Matrix Models

- Design PMM architectures tailored to this problem:
  - primary matrices as Hermitian functions of input features (e.g. Δt, G, variational parameters),
  - secondary matrices corresponding to effective observables (e.g. effective pairing Hamiltonian, pair occupation).
- Explore both:
  - eigenvalue-based PMMs (learning effective Hamiltonians),
  - observable-based PMMs (learning expectation values directly).
- Implement these PMMs in a numerical environment (Python/NumPy/PyTorch or similar), using the complex-valued gradient methods described in the PMM framework.

Objective 4: Zero-Error Trotter Step Extrapolation

- Train PMMs on simulated UCC data obtained at moderate Trotter step sizes Δt.
- Use the trained PMMs to extrapolate observables and energies to $\Delta t \to 0$.
- Compare PMM-based extrapolation with:
  - polynomial extrapolation,
  - standard neural network regressors (MLPs),

- other baseline methods (e.g. spline fits).

- Analyze the accuracy and stability of PMM extrapolations for:
  - ground-state energy,
  - occupation numbers and pairing gaps,
  - possibly time-dependent observables if time evolution is considered.

Objective 5: Performance Analysis and Physical Interpretation

- Quantify the efficiency of the PMM in terms of:
  - number of trainable parameters,
  - data requirements,
  - computational cost (training and inference).

- Investigate the analytic structure learned by the PMM (e.g. avoided crossings in effective spectra as functions of Δt or G).

- Discuss implications for near-term quantum devices and possible extensions to more complex Hamiltonians or ansätze.

4. Work Plan and Milestones (One-Year Timeline)

Semester 1 (Months 1–6)

Months 1–2: Literature Review and Theoretical Foundation

- Study the pairing Hamiltonian, UCC methods, and Trotter–Suzuki decompositions.

- Review PMM theory and the specific zero-error Trotter extrapolation example.

Deliverable: Written summary of theoretical background and key references.

Months 3–4: Classical Quantum Circuit Simulation

- Implement small pairing Hamiltonian instances and map them to qubit Hamiltonians.

- Build UCC ansätze tailored to pairing (e.g. pair excitation operators).

- Implement Trotterized UCC circuits in a simulator and generate benchmark data for energies and observables versus Δt.

Deliverable: Verified classical simulation code and initial dataset.

Months 5–6: PMM Architecture and Prototype

- Implement basic PMM architectures (Hermitian and unitary variants).

- Test PMMs on simplified regression tasks (e.g. emulating energies as functions of Δt for fixed parameters).

- Refine the choice of input features and PMM hyperparameters.

Deliverable: Working prototype PMM code and preliminary tests.

Semester 2 (Months 7–12)

Months 7–9: Full PMM Training and Extrapolation Studies

- Generate comprehensive datasets over a range of pairing strengths and UCC parameters.
- Train PMMs on Trotterized data and perform $\Delta t \to 0$ extrapolations.
- Systematically compare with polynomial and neural network extrapolations.

Deliverable: Trained PMM models and detailed numerical analysis of extrapolation quality.

Months 10–11: Performance Evaluation and Physical Interpretation

- Analyze the efficiency and robustness of PMMs.
- Investigate learned effective spectra and analytic properties.
- Explore potential extensions (e.g. different ansätze, other interaction channels).

Deliverable: Draft of results and discussion chapters for the thesis.

Month 12: Thesis Writing and Finalization

- Complete the thesis manuscript, including introduction, methods, results, and conclusions.
- Prepare the final oral presentation.

Deliverable: Final thesis document and defense presentation.

5. Expected Outcomes

- A complete computational framework for simulating Trotterized UCC circuits for the pairing Hamiltonian.
- A set of parametric matrix models tailored to zero-error Trotter step extrapolation in quantum simulations.
- Quantitative benchmarks comparing PMMs to standard extrapolation and machine learning approaches.
- Insight into how physics-informed matrix models can improve the reliability and interpretability of quantum algorithms for strongly correlated systems.

6. References

1. P. Cook, D. Jammooa, M. Hjorth-Jensen, D. D. Lee, *Parametric Matrix Models*, Nature Communications 16, 5929 (2025).

2. A. relevant review on unitary coupled cluster methods for quantum computing (to be added).

3. Standard references on the pairing Hamiltonian and reduced BCS models in nuclear physics and superconductivity (to be added).

4. Additional references on Trotter–Suzuki decompositions and NISQ-era quantum algorithms (to be added).