Master Thesis Project in Quantum Information Science and Technology

Parametric Matrix Models for Time-Dependent Hartree–Fock Dynamics

Duration: One Year (60 ECTS)

1. Introduction

Time-Dependent Hartree–Fock (TDHF) theory plays a central role in nuclear many-body physics, quantum chemistry, and ultracold atomic systems. It provides a mean-field description of the real-time evolution of an interacting quantum system using one-body density matrices. The TDHF equations,

$$i\hbar \frac{d}{dt}\rho(t) = [h[\rho(t)], \rho(t)],$$

describe nonlinear quantum dynamics where the single-particle Hamiltonian $h[\rho]$ depends self-consistently on the density matrix itself.

TDHF is a foundation for describing:

- nuclear collective motion,
- fission and fusion dynamics,
- giant resonances,
- real-time quantum evolution in cold-atom traps,
- mean-field quantum chemistry and time-dependent DFT.

Despite its utility, TDHF simulations are computationally demanding due to:

- large Hilbert-space dimension,
- nonlinear evolution,
- high cost of repeated time-stepping,
- sensitivity to parameter changes (interaction strengths, trap parameters, coupling constants).

Parametric Matrix Models (PMMs), introduced by Cook *et al.* (Nature Communications 16, 5929 (2025)), offer a physics-inspired surrogate modelling framework based on matrix equations. PMMs replace neural networks with parametric Hermitian or unitary matrices whose eigenvalues and eigenvectors generate outputs. Because the TDHF equations are themselves matrix differential equations with a strong operator algebra structure, PMMs provide a natural and theoretically motivated surrogate model for reduced-order TDHF dynamics.

This thesis aims to combine PMMs with TDHF to construct efficient, interpretable, reduced-basis models for real-time quantum many-body evolution.

2. Scientific Motivation

The TDHF equation describes the evolution of the density matrix $\rho(t)$ via a unitary propagator:

$$\rho(t+dt) = U(dt)\,\rho(t)\,U^\dagger(dt), \qquad U(dt) = \exp\left(-\frac{i}{\hbar}h[\rho(t)]\,dt\right),$$

with the Hamiltonian depending self-consistently on $\rho(t)$.

Solving TDHF requires:

- self-consistent construction of $h[\rho]$ at each time step,
- matrix exponentiation at each time step,
- numerical stability control for long-time simulations.

For parameter sweeps (e.g., different coupling constants, nuclear shapes, trap strengths, interaction terms), full TDHF simulations are extremely costly.

PMMs offer several advantages:

- the ability to emulate unitary time evolution;
- analytic continuation of dynamics into the complex plane;
- built-in preservation of unitarity and Hermiticity;
- significant reduction in model size vs. neuron-based models;
- direct embedding of operator commutation relations.

The central hypothesis is that PMMs can reproduce TDHF trajectories as implicit functions of interaction parameters and initial conditions—offering a fast surrogate model that still respects the operator structure and physical constraints.

3. Objectives of the Thesis

Objective 1: Theory of TDHF and PMMs

- Study the TDHF equations for selected quantum systems (nuclear, atomic, or simplified models). We will start with the simpler Lipkin model.
- Review the theory of PMMs, including Hermitian and unitary forms.
- Understand the analytic gradient evaluation described by Cook *et al.*

Objective 2: Numerical TDHF Solver and Data Generation

- Implement a standard TDHF solver using:
  - explicit or implicit Runge–Kutta,
  - Crank–Nicolson,
  - Magnus expansion,

  - or a split-operator method.

- Generate trajectory datasets (density matrices, expectation values, observables).
- Explore simple test systems:
  - Lipkin-Meshkov-Glick (LMG) model,
  - Two-level pairing models,
  - Harmonic oscillator trap with mean-field interactions,
  - Eventually, study small Hubbard or spin-chain systems.

Objective 3: PMM Construction for Time Evolution

- Build a PMM where:
  - primary matrices mimic the structure of the effective Hamiltonian,
  - unitary primary matrices mimic the TDHF propagator,
  - secondary matrices encode observables of interest.
- Investigate affine PMMs and multiplicative (unitary) PMMs.
- Embed commutation relations of the many-body Hamiltonian as constraints.

Objective 4: Training and Optimization

- Train PMMs to reproduce TDHF trajectories as functions of:
  - interaction strengths,
  - coupling constants,
  - initial conditions,
  - model parameters (e.g., pairing strength, trap frequency).
- Use analytic gradients and unitary transformations for optimization.
- Investigate overfitting, stability, and extrapolation behavior.

Objective 5: Benchmarking and Validation

- Compare PMMs against:
  - full TDHF solver,
  - recurrent neural networks (LSTMs / GRUs),
  - in collaboration with other students study physics-informed neural networks,
  - reduced-basis TDHF methods (eigenvector continuation).
- Evaluate accuracy over time, error accumulation, and conservation laws:
  - norm conservation,
  - energy conservation,
  - particle number.

Objective 6: Possible Extensions

- PMM emulation of TDHF linear-response spectra.
- PMM acceleration of TDHF in higher dimensions.

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

Semester 1 (Months 1–6)

Months 1–2: Theory and Background

- Study TDHF theory and typical numerical implementations.
- Study PMM theory in detail.
- Select model systems (e.g., LMG, two-level systems, small Hubbard chain).

Deliverable: Literature review on TDHF and PMMs.

Months 3–4: TDHF Solver and Dataset Production

- Implement TDHF solvers for selected systems.
- Test convergence in time step and basis size.
- Generate data for a range of coupling constants and initial states.

Deliverable: Verified TDHF solver and dataset.

Months 5–6: PMM Architecture Development

- Construct PMMs for time evolution.
- Test small (e.g., $n = 5$ or $n = 7$) matrices on short trajectories.
- Integrate analytic gradients.

Deliverable: First working PMM reproducing basic TDHF trajectories.

Semester 2 (Months 7–12)

Months 7–9: Full PMM Training and Stability Analysis

- Train PMMs over large parameter domains.
- Evaluate long-time stability and conservation laws.
- Study spectrum and analytic structure of PMM primary matrices.

Deliverable: Fully trained PMM for TDHF dynamics.

Months 10–11: Benchmarking and Comparisons

- Compare PMMs with NN-based surrogates and reduced-basis TDHF.

- Produce tables/plots of accuracy, stability, and computational cost.

Deliverable: Comprehensive benchmarking report.

Month 12: Writing and Final Submission

- Write and revise the full thesis manuscript.
- Prepare the final oral presentation.

Deliverable: Completed thesis and defense presentation.

5. Expected Outcomes

- A full TDHF simulation code and dataset.
- A PMM-based surrogate model for nonlinear quantum time evolution.
- Demonstrated parameter-efficiency of PMMs relative to neural networks.
- Insight into embedding physical constraints directly into machine learning architectures.
- A complete master thesis document summarizing theory, methods, and results.

6. References

1. P. Cook, D. Jammooa, M. Hjorth-Jensen, D. D. Lee, *Parametric Matrix Models*, Nature Communications 16, 5929 (2025).
2. P. Ring and P. Schuck, *The Nuclear Many-Body Problem.*
3. K. Hagino and Y. Tanimura, reviews on TDHF and nuclear dynamics.
4. Additional references to be added as appropriate.