Intern projects 2026

Roeland Wiersema

Riemannian Hessians for Neural Quantum States

The quantum geometric tensor determines several geometric aspects of Neural Quantum States. The real part of this tensor gives a metric, which can be used to perform a Riemannian gradient flow (Stochastic Reconfiguration/Natural Gradient Descent) for ground state searches. The imaginary part enables the time evolution of a neural quantum state through a symplectic flow (t-VMC). In this project we will study another geometric object: the Riemannian Hessian. This object can be estimated in a similar fashion to the quantum geometric tensor but contains much richer geometric information that will allow us to study the curvature of the variational manifold, construct geodesics and perform parallel transport. Applicants do not require extensive knowledge of differential geometry, but some programming experience in JAX/Netket will be useful.

Jason Kaye

Analytic continuation from high-accuracy deterministic impurity solvers in dynamical mean-field theory calculations

The problem of recovering the real-frequency spectral function from the imaginary time Green's function is severely ill-conditioned. However, recent developments in analytic continuation (AC) schemes, as well as methods of computing imaginary time data with high accuracy, create an opportunity to revisit the practicality of AC in the context of dynamical mean-field theory (DMFT) calculations. On the one hand, numerical results from recently-introduced AC schemes [1] suggest the possibility of systematic convergence; as the accuracy of the imaginary time data improves, so does the accuracy of the recovered spectral function (with a loss of precision due to conditioning). On the other hand, unlike for typical quantum Monte Carlo based methods such as CT-HYB, deterministic imaginary time DMFT impurity solvers have been proposed which have the possibility of producing imaginary time data with high-order accuracy (perhaps within a given approximation) and no stochastic noise. Examples include a new

solver based on perturbation theory and high-order accurate sum-of-exponentials representations [2], and tensor network-based solvers. This project will explore the combination of these two developments, and compare the reliability of AC in this context with the typical scenario of AC from noisy quantum Monte Carlo data.

[1] L. Zhang, Y. Yu, E. Gull, "Minimal pole representation and controlled analytic continuation of Matsubara response functions", Phys. Rev. B, 110, 035154 (2024).
[2] Z. Huang, D. Golež, H. U. R. Strand, J. Kaye, "Automated evaluation of imaginary time strong coupling diagrams by sum-of-exponentials hybridization fitting", SciPost Phys., 19, 121 (2025).

Miguel Morales, Shiwei Zhang

Internship in quantum Monte Carlo at CCQ

Our work involves the development of algorithms and codes for quantum systems using stochastic approaches, and their application to tackle important problems in physics and chemistry. We have a number of projects appropriate for internships, focusing on methodology, software, or applications. CCQ has a dynamic environment with many other members working on related problems. We welcome you to suggest/propose projects which can create synergy with us.

1. Properties of ultracold atoms in optical lattices. The goal is to perform accurate calculations to predict various correlations in these systems which are being realized with exquisite control in various laboratories. There are several possible projects here involving either finite-temperature or ground-state calculations. They employ auxiliary-field quantum Monte Carlo coupled self-consistently to gauge constraints using mean-field calculations. So an internship project could be configured to focus on different aspects.

2. Developments and applications of auxiliary-field quantum Monte Carlo. There are several projects involving the development and application of this technique in the study of properties of correlated systems, including

Hubbard models and Morie materials. Possible projects include the development of novel trial wavefunctions for AFQMC using variational neural quantum states, extensions of finite-temperature AFQMC to Moire materials and applications of AFQMC to Moire continuum Hamiltonians.

Riccardo Rende, Shiwei Zhang

A Python Framework for Neural Quantum States in Green's Function Monte Carlo

We propose a summer internship focused on developing a lightweight, user-friendly Python package that allows users to define a Neural Quantum State (NQS) as a Python function and run Green's Function Monte Carlo (GFMC) simulations with it. Because NQS models can accurately capture the sign structure of many-body wavefunctions, we expect this approach to integrate effectively with GFMC and enable robust simulations across a broad range of systems. This project is well scoped for a motivated intern with interests in numerical methods, quantum many-body physics, and scientific software development.

[1] Quantum Monte Carlo Approaches for Correlated Systems, F. Becca and S. Sorella, Cambridge University Press
[2] Transformer variational wave functions for frustrated quantum spin systems, L.L. Viteritti, R. Rende and F. Becca, PRL 130 (23) 236401

Chia-Nan Yeh

Ab initio many-body perturbation theory for solids and molecules using interpolative separable density fitting

The project focuses on developing many-body perturbation theory (such as GW) for solids and molecular systems within the interpolative separable density fitting framework. Students will work with numerical algorithms, run many-body electronics structure calculations, analyze results, and contribute targeted improvements to the workflow. Prior background in first-principles electronic structure methods is encouraged.