Machine learning and artificial intelligence for quantum-mechanical systems

Master of Science thesis project

November 2024

1 Scientific aims

The aim of this master of science project is to develop many-body theories for studies of strongly interacting quantum mechanical many-particle systems using novel methods from deep learning theories, in particular advanced neural networks and other generative models.

For interacting many-particle systems where the degrees of freedom increase exponentially, quantum mechanical many-body methods like quantum Monte Carlo methods, Coupled Cluster theory, Green's function theories, density functional theories and other, play a central role in understanding experiments in a wide range of fields, spanning from atomic and molecular physics and thereby quantum chemistry to condensed matter physics, materials science, nano-technologies and quantum technologies and finally processes like fusion and fission in nuclear physics. This list is definitely not exhaustive as the are many other areas of applications for quantum mechanical many-body theories.

Quantum Monte Carlo techniques are widely applicable and have been used in studies of a large range of systems. The main difficulty with QMC calculations of fermionic systems is ensuring the fermionic antisymmetry is respected. In Diffusion Monte Carlo calculations, which in principle yield the exact solutions in the limit of lon simulation times, the prescription to ensure this is fixing the nodes of the system to prevent the large errors that would come with the summation of alternating signs. Unfortunately this prescription is not variational in nature and can in some cases result in convergence to energies lower than the true ground state of the system. This is one of the advantages of VMC calculations since they are known to be variational the resulting wavefunction will always have an energy larger than or equal to the true ground state wavefunction.

The problem with variational Monte Carlo calculations has been the choice of trial wave function. Recently, several research groups have introduced, with great success, neural networks as a way to represent the trial wave function. Recent works on infinite nuclear matter[1, 3], the unitary Fermi gas [2], and Daniel Haas Beccatini's recent master of science thesis project [4] have shown that one can obtain results of equal accuratness as the theoretical benchmark calculations provided by diffusion Monte Carlo results. This has opened up a new area of research and the present thesis project aims at developing further deep learning approaches to the studies of strongly interacting many-body systems.

The plans here are to extend the studies in [4] to studies of low-dimensional systems such as quantum dots and the infinite electron gas in two dimensions. These are systems of great interest for materials science studies, nanotechnologies and quantum technologies. A proper understanding of the properties of such systems will play a crucial role in designing for example quantum gates and circuits. These systems are studied experimentally at the university of Oslo at the Center for Materials Science and Nanotechnologies (SMN). The theoretical activity at the Center for Computing in Science Education and the Computational Physics research group have through the last years developed a strong collaboration with several researchers at the SMN.

The thesis of Daniel Haas Beccatini [4] with codes and additional material will serve as an excellent backgroun material.

The plan for this thesis project is as follows:

- Spring 2025: follow courses and get familair with Monte Carlo methods and how to use neural networks to solve simpler quantum mechanical. The software developed in [4] can serve as a guidance for developing own code.
- Fall 2025: Include stochastic resampling [4] and develop code for studies of both bosonic and fermionic systems.
- Spring 2026: Apply formalism and code to studies of two-dimensional systems like quantum dots and/or the infinite electron gas in two dimensions. Finalize thesis by May 2026.

References

[1] Bryce Fore, Jane M. Kim, Giuseppe Carleo, Morten Hjorth-Jensen, Alessandro Lovato, and Maria Piarulli, Dilute neutron star matter from neural-network quantum states, Physical Review Research **5**, 033062 (2023) and `https://journals.aps.org/prresearch/abstract/10.1103/PhysRevResearch.5.033062`

[2] Jane Kim, Gabriel Pescia, Bryce Fore, Jannes Nys, Giuseppe Carleo, Stefano Gandolfi, Morten Hjorth-Jensen, Alessandro Lovato, Neural-network quantum states for ultra-cold Fermi gases, Nature Communications Physics **7**, 148 (2024) and `https://www.nature.com/articles/s42005-024-01613-w`

[3] Bryce Fore, Jane Kim, Morten Hjorth-Jensen, Alessandro Lovato, Investigating the crust of neutron stars with neural-network quantum states,

Nature Communications Physics in press and https://arxiv.org/abs/2407.21207

[4] Daniel Haas Beccatini, Master of Science thesis, University of Oslo, 2024, Deep Learning Methods for Quantum Many-body Systems, A study on Neural Quantum States, https://www.duo.uio.no/handle/10852/113984