Deep Learning and Quantum Many-body problems

Master of Science thesis project

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Introduction and overview

Predicting the structure of quantum many-body systems from first principles in quantum mechanics is a central challenge in physics, chemistry, and material science. Deep learning techniques have recently proven to be powerful tools for solving interacting quantum mechanical problems in condensed matter physics, atomic and molecular physics and quantum chemistry, nuclear physics and materials science.

The above implies solving the Schrödinger equation for systems of many interacting bosons or fermions. This is classified as an NP-hard problem due to the complexity of the required many-dimensional wave function, resulting in an exponential growth of degrees of freedom. Reducing the dimensionalities of quantum mechanical many-body systems is an important aspect of modern physics, ranging from the development of efficient algorithms for studying many-body systems to exploiting the increase in computing power. To write software that can fully utilize the available resources has long been known to be an important aspect of these endeavors. Despite tremendous progress has been made in this direction, traditional many-particle methods, either quantum mechanical or classical ones, face huge dimensionality problems when applied to studies of systems with many interacting particles.

Over the last two decades, quantum computing and machine learning have emerged as some of the most promising approaches for studying complex physical systems where several length and energy scales are involved. Machine learning techniques and in particular neural-network quantum states [Goodfellow *et al.*(2016)Goodfellow, Bengio, and Courville] have recently been applied to studies of many-body systems, see for example Refs. [Carleo and Troyer(2017), Carrasquilla and Torlai(2021), Pfau *et al.*(2020)Pfau, Spencer, Matthews, and Foulkes, Calcavecchia *et al.*(2014)Calcavecchia, Pederiva, Kalos, and Küh Carleo *et al.*(2019)Carleo, Cirac, Cranmer, Daudet, Schuld, Tishby, Vogt-Maranto, and Zdeborová, Boehnlein *et al.*(2022 Adams *et al.*(2021)Adams, Carleo, Lovato, and Rocco, Lovato *et al.*(2022)Lovato, Adams, Carleo, and Rocco], in various fields of physics and quantum chemistry, with very promising results. In many of these studies, one has obtained results that align well with exact analytical solutions or are in close agreement with state-of-the-art quantum Monte Carlo calculations.

The variational and diffusion Monte Carlo algorithms are among the most popular and successful methods available for ground-state studies of quantum mechanical systems. They both rely on a suitable ansatz for the ground-state of the system, often dubbed *trial wave function*, which is defined in terms of a set of variational parameters whose optimal values are found by minimizing the total energy of the system. Devising flexible and accurate functional forms for the trial wave functions requires prior knowledge and physical intuition about the system under investigation. However, for many systems we do not have this intuition, and as a result it is often difficult to define a good ansatz for the state function.

According to the universal approximation theorem, a deep neural network can represent any continuous function within a certain error [Hornik *et al.*(1989)Hornik, Stinchcombe, and White] — see also Refs. [Murphy(2012), Hastie *et al.*(2009)Hastie, Tibshirani, and Friedman, Bishop(2006), Goodfellow *et al.*(2016)Goodfell for further discussions of deep leaning methods. Since the variational state wave function in principle can take any functional form, it is natural to replace the trial wave function with a neural network

and treat it as a machine learning problem. This approach has been successfully implemented in recent works, see for example Refs. [Pfau *et al.*(2020)Pfau, Spencer, Matthews, and Foulkes, Carleo and Troyer(2017), Cassella *et al.*(2022)Cassella, Sutterud, Azadi, Drummond, Pfau, Spencer, and Foulkes, Adams *et al.*(2021)Adams, Carle Lovato *et al.*(2022)Lovato, Adams, Carleo, and Rocco], and forms the motivation for the present study. Here, the neural network of choice was derived from so-called restricted Boltzmann machines, much inspired by the recent contributions by Carleo *et al.*, see for example Refs. [Carleo and Troyer(2017), Carleo *et al.*(2019)Carleo, Cirac, Cranmer, Daudet, Schuld, Tishby, Vogt-Maranto, and Zdeborová]. Note that neural-networks representations of variational states are more general, as they do not in principle require prior knowledge on the ground-state wave function, thereby opening the door to systems that have yet to be solved. Particular attention however has to be devoted to the symmetries of the problem, whose inclusion is critical to achieve accurate results..

Thesis Project

The aim here is to study systems of confined fermions and bosons in one and two dimensions. Strongly confined electrons offer a wide variety of complex and subtle phenomena which pose severe challenges to existing many-body methods. Quantum dots in particular, that is, electrons confined in semiconducting heterostructures, exhibit, due to their small size, discrete quantum levels. The ground states of, for example, circular dots show similar shell structures and magic numbers as seen for atoms and nuclei. These structures are particularly evident in measurements of the change in electrochemical potential due to the addition of one extra electron.

Small confined systems, such as quantum dots (QD), have become very popular for experimental study. Beyond their possible relevance for nanotechnology, they are highly tunable in experiments and introduce level quantization and quantum interference in a controlled way.

Similarly, other fermionic systems like atoms, molecules, nuclei, the infinite homogeneous electron gas and infinite nuclear matter, are all systems which can be studied with the same many-body methods. Thus, a proper theoretical understanding of such systems requires the development of appropriate and reliable theoretical few- and many-body methods. Furthermore, for say quantum dots with more than two electrons and/or specific values of the external fields, this implies the development of few- and many-body methods where uncertainty quantifications are provided. For most methods, this means providing an estimate of the error due to the truncation made in the single-particle basis and the truncation made in limiting the number of possible excitations. For systems with more than three or four electrons, **ab initio** methods that have been employed in studies of quantum dots are variational and diffusion Monte Carlo, path integral approaches, large-scale diagonalization (full configuration interaction and to a more limited extent coupled-cluster theory. Exact diagonalization studies are accurate for a very small number of electrons, but the number of basis functions needed to obtain a given accuracy and the computational cost grow very rapidly with electron number. In practice they have been used for up to eight electrons, but the accuracy is very limited for all except $N \leq 3$. Monte Carlo methods have been applied up to $N \sim 100$ electrons. Diffusion Monte Carlo, with statistical and systematic errors, provide, in principle, exact benchmark solutions to various properties of quantum dots. However, the computations start becoming rather time-consuming for larger systems. Mean field methods like various Hartree-Fock approaches and/or current density functional methods give results that are satisfactory for a qualitative understanding of some systematic properties. However, comparisons with exact results show discrepancies in the energies that are substantial on the scale of energy differences. The above-mentioned many-body methods all experience what is the loosely called the *curse of dimensionality*. This means that the increased number of degrees freedom hinders the application of most first principle methods. As an example, for direct diagonalization methods, Hamiltonian matrices of dimensionalities larger than ten billion basis states, are simply computationally intractable. Such a dimensionality translates into few interacting particles only. For larger systems one is limited to much more approximative methods. Reecent approaches in Machine Learning as well as in quantum computing, hold promise however to circumvent partly the above problems with increasing degrees of freedom.

The specific aim of this thesis topic is to, based on quantum Monte Carlo methods, to explore deep learning approaches to many-body systems based on neural networks, see the recent work of for example Adams et al..

Specific tasks and milestones. The specific task here is to implement and study deep learning methods for solving quantum mechanical many-particle problems of fermions. The results can be easily compared with exisiting standard many-particle codes developed by former students at the Computational Physics group. These codes will serve as useful comparisons in order to gauge the appropriateness of recent Machine Learning approaches to quantum mechanical problems.

The basic framework to be developed contains:

1. The development of a Variational Monte Carlo code for fermions.
2. The development of a trial wave function for the correlated part based on deep neural networks.
3. Be able to study quantum mechanical systems with interactions for bosons and fermions in one and two dimensions.
4. Compare results with those obtained with recent libraries like FermiNet, SchNet and other.

The milestones are

1. Spring semester 2023: Develop a Variational Monte Carlo framework for fermions without a self-consistent single-particle basis. Parts of this will be done in the course FYS4411, Computational Quantum Mechanics.
2. Fall semester 2023: Introduce neural networks for the correlated part of the trial wave function used in Monte Carlo studies. Study simpler Hamiltonians in one and two dimensions like those described in [1, 2].
3. Spring semester 2024: Perform numerical studies of quantum systems involving quantum dots in two dimensions and compare with results from other libaries.
4. Spring semester 2024: Final thesis

The thesis is expected to be handed in May/June 2024.

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[Note1()] Natural units are used with energy given in units of $\hbar$ and length given in units of $\sqrt{\hbar/m}$.

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