Machine Learning, Deep learning and Quantum Mechanics

Master of Science thesis project

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Machine Learning and the Quantum Many-body Problem

Solving quantum mechanical problems for atoms, molecules, materials, and interfaces is of fundamental importance to a large number of disciplines including physics, chemistry, and materials science. Since the early development of quantum mechanics, it has been noted, by Dirac among others, that *...approximate, practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.*

Historically, this has meant invoking approximate forms of the underlying interactions (mean field, tight binding, etc.) or relying on phenomenological fits to a limited number of either experimental observations or theoretical results (e.g., force fields). The development of feature-based models is not new in the scientific literature. Indeed, prior even to the acceptance of the atomic hypothesis, van der Waals argued for an equation of state based on two physical features. Machine learning (i.e., fitting parameters within a model) has been used in physics and chemistry since the dawn of the computer age. The term machine learning is new; the approach is not.

More recently, high-level ab initio calculations have been used to train artificial neural networks to fit high-dimensional interaction models and to make informed predictions about material properties.

Machine learning can also be used to accelerate or bypass some of the heavy machinery of the ab initio method itself. In the work of Snyder et al, the authors replaced the kinetic energy functional within density-functional theory with a machine-learned one, *learned* the mappings from potential to electron density and from charge density to kinetic energy, respectively.

Thesis Projects

Here we present possible theses paths based on Machine Learning and studies of quantum mechanical systems. Possible systems are fermion or boson systems

where the quantum mechanical particles are confined to move in various types of traps. A typical example which one could start with is to study a system of one and two electrons in two or three dimensions whose motion is confined by a harmonic oscillator potential. This system has, for one and two electrons only in two or three dimensions, analytical solutions for the energy and the state functions.

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 deeep 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.

Four recent articles (see below) have shown the reliability of these methods and the aim is to study and implement some of these algorithms to first a system of one electron moving in a confining potential. Thereafter we switch to the interacting two-electron and many-electron problems and apply these algorithms. We will focus first on systems of quantum dots, but the codes can easily be extended to systems of atoms and molecules.

The basic framework to be developed contains:

1. The determination of a self-consistent single-particle basis using the Hartree-Fock method.

2. The development of a Variational Monte Carlo code for fermions. If time allows, excursions into diffusion Monte Carlo are also possible.

3. The development of a trial wave function for the correlated part based on deep neural networks.

The milestones are

1. Spring semester 2021: 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 2021: Develop a code for a self-consistent single-particle basis using the Hartree-Fock method. The code should be flexible enough to handle different types of interacting fermionic systems.

3. Fall semester 2021: Introduce neural networks for the correlated part of the trial wave function used in Monte Carlo studies.

4. Spring semester 2022: Perform numerical studies of different quantum mechanical systems. Study weakly correlated and strongly correlated fermionic systems, ground state properties and correlation functions like two-body densities.

5. Spring semester 2022: Final thesis

The thesis is expected to be handed in May/June 2022.

References. Highly relevant articles for possible thesis projects are:

1. Carleo and Troyer

2. Mills et al

3. Pfau et al, Ab-Initio Solution of the Many-Electron Schrödinger Equation with Deep Neural Networks

4. Adams et al., Variational Monte Carlo calculations of $A \leq 4$ nuclei with an artificial neural-network correlator ansatz.

5. See also Recent advances and applications of machine learning in solid-state materials science, by Jonathan Schmidt et al