Machine Learning, Deep learning and Quantum Mechanics, a Focus on Recurrent Neural Networks

Master of Science thesis project

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Machine Learning and the Quantum Many-body Problem

The aim of this thesis project is to employ and develop Recurrent neural networks and similar deep learning algorithms for studies of many interacting particles. The thesis project can be combined with the inclusion of more traditional many-body methods like coupled cluster theory, large-scale eigenvalue methods and in-medium similarity renormalization group theory.

Typical systems which can be studied are strongly confined electrons. These systems 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. Beyond their possible relevance for nanotechnology, they are highly tunable in experiments and introduce level quantization and quantum interference in a controlled way. Other systems of great interest (and which are similar in terms of interaction models) is the infinite homogeneous elctron gas in two and three dimensions.

A proper theoretical understanding of such systems requires the development of appropriate and reliable theoretical few- and many-body methods. 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 pertinent statistical 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.

Other systems of interest are studies of infinite systems such as the homogeneous electron gas and/or infinite nuclear matter. The latter is a widely popular many-body system, with far ranging consequences and interests, from the structure of neutron stars to a deeper understanding of neutrino oscillations.

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 aim of this thesis project is thus to explore various Machine Learning approaches.

Specific tasks and milestones. The specific task here is to implement and study recently developed deep learning algorithms based on neural networks and in particular on recurrent neural networks for solving quantum mechanical many-particle problems. 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 aim here is to use recurrent neural networks (RNNs) to study quantum mechanical many-body methods like the family of similarity renormalization group methods. This method is a rewrite of many-body equations in terms of coupled ordinary differential equations, see chapter 10 of Lecture Notes in Physics vol. 936.

The projects can easily be split into several parts and form the basis for collaborations among several students. The milestones are as follows:

1. Spring 2020: Develop a code for solving the Schroedinger equation for one and two particles in 1, 2 and 3 dimensions using recurrent neural networks and the Similarity Renormalization Group method. Compare the results to exact numerical diagonalization of the same systems.

2. Fall 2020: Extend the project to include the in-medium similarity renormalization group method and develop an RNN based code for handling many-particle systems.

3. Spring 2021: The choice of systems here is optional. Examples could be the quantum dot systems mentioned above or the homogenoeus electron gas. Such calculations have never been performed before and can lay the foundaton for several scientific articles.

The thesis is expected to be handed in May/June 2021.

References. Highly relevant articles for possible thesis projects are:

1. Hergert et al, chapter 10 in particular
2. Mills et al
3. Pfau et al, Ab-Initio Solution of the Many-Electron Schrödinger Equation with Deep Neural Networks
4. See also Recent advances and applications of machine learning in solid-state materials science, by Jonathan Schmidt et al