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

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. The aim here is to use Recurrent neural networks to study the solutions of eigenvalue problems.

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, $\Delta_N = \mu(N+1) - \mu(N)$. Here N is the number of electrons in the quantum dot, and $\mu(N) = E(N) - E(N-1)$ is the electrochemical potential of the system. Theoretical predictions of Δ_N and the excitation energy spectrum require accurate calculations of ground-state and of excited-state energies. 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.

A proper theoretical understanding of such systems requires the development of appropriate and reliable theoretical few- and many-body methods. Furthermore, for 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 aim of these thesis topics aim thus at exploring various Machine Learning approaches.

Specific tasks and milestones. The specific task here is to implement and study the recently developed deep learning algorithms 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 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.

2. Fall 2020: Extend the project to include the in-medium similarity renormalization group method.

3. Spring 2021: Extend to studies of the homogenoeus electron gas.

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