Quantum Computing and Many-Particle Problems

Master of Science thesis project

Jan 22, 2018

Quantum 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. Similarly, algorithms from Quantum Computing hold now great promise for sovling quantal many-particle problems.

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.

Quantum Computing and Machine Learning

Quantum Computing and Machine Learning are two of the most promising approaches for studying complex physical systems where several length and energy scales are involved. Traditional many-particle methods, either quantum mechanical or classical ones, face huge dimensionality problems when applied to studies of systems with many interacting particles. To be able to define properly effective potentials for realistic molecular dynamics simulations of billions or more particles, requires both precise quantum mechanical studies as well as algorithms that allow for parametrizations and simplifications of quantum mechanical results. Quantum Computing offers now an interesting avenue, together with traditional algorithms, for studying complex quantum mechanical systems. Machine Learning on the other hand allows us to parametrize these results in terms of classical interactions. These interactions are in turn suitable for large scale molecular dynamics simulations of complicated systems spanning from subatomic physics to materials science and life science.

In addition, **Machine Learning** plays nowadays a central role in the analysis of large data sets in order to extract information about complicated correlations. This information is often difficult to obtain with traditional methods. For example, there are about one trillion web pages; more than one hour of video is uploaded to YouTube every second, amounting to 10 years of content every day; the genomes of 1000s of people, each of which has a length of 3.8×10^9 base pairs, have been sequenced by various labs and so on. This deluge of data calls for automated methods of data analysis, which is exactly what machine learning provides. Developing activities in these frontier computational technologies is thus of strategic importance for our capability to address future science problems.

The problems we target satisfy the dual criteria of being integral to the fundamental understanding of complex physical systems and also compelling a major conceptual advance in method or theory with broad applications to other science fields.

Thesis Projects

Here we present possible theses paths based on Quantum Computing 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, $\Delta_N = \mu(N+1) - \mu(N)$. 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. Recent approaches in Quantum Computing (and Machine Learning as well) hold promise however to circumvent partly the above problems with increasing degrees of freedom. The aim of these thesis topics aim thus at exploring Quantum Computing algorithms for solving quantal many-particle problems.

Specific tasks and milestones. The specific task here is to implenent and study Quantum Computing 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 Quantum Computing approaches to quantum mechanical problems.

Recent scientific articles (see below) have shown the reliability of these methods and the aim is to study and implement these algorithms to first a system of one electron moving in a confining potential. Thereafter we switch to the interacting two-electron, many-electron and many-boson problems and apply these algorithms. One can also study other machine learning algorithms.

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

1. Fall 2XXX: Based on the works of Dumitrescu et al solve the non-interacting case for a system of N non-interacting bosons and fermions.

2. Spring 2XXX: Extend to systems of many interacting bosons and fermions and finalize thesis.