Quantum Computing and Many-Particle Problems

Master of Science thesis project

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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.

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. Recent scientific articles have shown the reliability of these methods on existing and real quantum computers, see for example Dumitrescu et al.

Here the focus is first on tailoring a Hamiltonian like the pairing Hamiltonian and/or Anderson Hamiltonian in terms of quantum gates, as done by Ovrum and Hjorth-Jensen.

Reproducing these results will be the first step of this thesis project. The next step includes adding more complicated terms to the Hamiltonian, like a particle-hole interaction as done in the work of Hjorth-Jensen et al.

The final step is to implement the action of these Hamiltonians on existing quantum computers like Rigetti's Quantum Computer.

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: Study and write a program to reproduce the pairing model results of Ovrum and Hjorth-Jensen using the the **quantum phase estimation algotrithm**.

2. Fall 2020: Add more complicated terms to the Hamiltonian and rewrite these in terms of quantum gates. Write program to compute expectation values and compare with other many-body methods like exact diagonalization methods. The addition of variational quantum eigensolver (VQE) should also be implemented and compared with the phase estimation algorithm.

3. Spring 2021: Finalize thesis project and study other quantum mechanical methods and systems.

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

Additional Literature.

1. The :Github repository":"https://github.com/mhjensen/QuantumComputing" contains additional information, codes, articles and textbooks on quantum computing and quantum information theory.

2. The Whitebook on Quantum Computing for the Nuclear Many-body problem, see the **whitepaper** link contains many interesting articles and links.