Time Evolution of Quantum Mechanical systems

Implementation of Time-Dependent Coupled Cluster methods

Master of Science thesis project

November 2022

Introduction and overview

The aim of this project is the study of time evolution in fermionic systems through the use of quantum many-body theory. Quantum many-body theory has provided methods to solve problems in such diverse areas as atomic, molecular, solid-state and nuclear physics, chemistry and materials science. In the past decades, static properties such as binding energies and various expectation values have been calculated. The introduction of time in these calculations yields an insight into the dynamics of quantum mechanical systems, such as the electron behavior under an external potential in quantum dots and the consolidation of composite systems undergoing nuclear fusion. Specifically, the goal is to implement the time dependent version of the Coupled Cluster approach [1, 2, 5, 3, 4], a method containing a plethora of desired properties such as size consistency and extensivity. The results can be compared with exisiting codes using time-dependent full configuration interaction theory [6, 7].

General introduction to possible physical systems.

The code developed during this thesis will be written in such a way that different fermionic system can be handled. Examples of potential applications are ions confined in various traps [8]. 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.

Application in nuclear physics might also be of interest[5], where the Coupled Cluster method was originally introduced. In particular, the process of two α-particles fusing into Beryllium ($^4_2\mathrm{He} + ^4_2\mathrm{He} \rightarrow ^8_4\mathrm{Be}$) could serve as the ultimate goal of the thesis, being part of the tripe-alpha process, the backbone of stellar nucleosynthesis.

Specific tasks and milestones

The specific task here is to study the time evolution of quantum mechanical systems using the Coupled Cluster (CC) method, in order to be able to study the time evolution of an interacting quantum mechanical system. In order to achieve this, the following milestones outline the thesis:

1. Spring 2023: Start writing a time-independent Coupled Cluster code with double excitations first following [4] and applied to a small confined fermionic system in one dimension. Here we have in mind electrons confined in harmonic oscillator traps [9] and/or the Calogero-Sutherland

[10] type of Hamiltonians which provide analytical answers to many-body problems. Singles excitations can be added later. Finalize remaining courses.

2. Fall 2023: Extend the program from spring 2023 to include singles excitations and time-dependence without time-dependence for single-particle orbitals, see Ref. [5]. Compare with existing results obtained with full configuration theory as done in [6, 7].

3. Spring 2024: Extend the program to include time-dependence of the single-particle orbitals and compare with corresponding full configuration theory calculations. Apply to systems of quantum dots and/or the fusion of two α-particles. Finalize thesis and present final results.

The thesis is expected to be handed in May/June 2024

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