Master Thesis project

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Master Thesis - Project Description Tentative title: **Time-dependent many-body methods for quantum technologies**

1 Background

The aim of this project is the study of time evolution in fermionic systems through the use of quantum many-body theory applied to candidate systems for realizing quantum circuits and gates. In particular we will analyze and study properties like the time evolution of entanglement and how to realize quantum gates for systems of electrons confined in one, two and three dimensions, so-called quantum dot systems [1].

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 [1]. Specifically, the goal here is to develop a computational framework (codes and theory) for studies of interacting systems of electrons with time-dependence using time-dependent full configuration interaction theory [2, 3].

Based on the theoretical solutions and design of specific quantum gates, the final aim is to study the simulation of systems of specific quantum circuits as function of time. The aim is to simulate systems of two to several electrons confined in various potential traps [5].

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.

Recently, several experimental groups have started to study how one can use confined eletrons to make quantum gates and circuits in order to implement different quantum computing algorithms. To study their feasibility using quantum mechanical simulation tools like time-dependent many-body methods can hopefully shed light on such candidate systems. Furthermore, the design of circuits and systems to simulate will include algorithms from quantum computing like the Variational Quantum Eigensolver [6].

This thesis will also include the utilization of efficient single-particle computational basis sets from density functional theories. These basis sets allow for the inclusion of specific medium-dependent properties and can thus be closely linked with experimental work conducted at the center for Materials Science and Nanotechnology (SMN) at the University of Oslo. The Computational Physics group at the University of Oslo works closely with experimentalists at the SMN and at Michigan State University, with the aim to develop a theoretical quantum engineering platform that describes in the best possible way experimental realizations of various quantum gates and circuits.

2 Project Tasks and Tentative Timeline

1. Spring 2024: Start writing a time-dependent Hartree-Fock code applied to a system of two electrons in one dimension in one and thereafter two harmonic oscillator traps. Here we have in mind electrons confined in harmonic oscillator traps as done by the authors of Ref. [4]. Finalize remaining courses.

2. Spring 2024: Extend these studies to include single-particle basis functions from density functional theory.

3. Fall 2024: Extend the program from spring 2024 to study time-dependent full configuration interaction [2, 3] and study systems of two and up to four interacting electrons in one or more harmonic oscillator traps. Study the time-evolution of entanglement for these systems based on the recent work of the Computational Physics group [5].

4. Spring 2025: Extend the program to include the simulation of specific quantum circuits and the stability of such systemsbased on the Variational Quantum Eigensolver algorithm [6]. Here one can think of devising various quantum gates like CNOT, iSWAP gates and other and study the feasibility of such quantum circuits.

The thesis is expected to be handed in May/June 2025

References

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