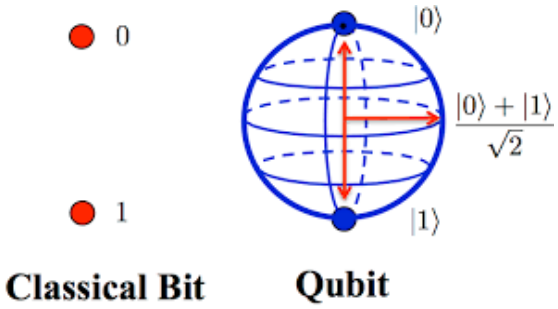
CHALMERS UNIVERSITY OF TECHNOLOGY

Master's Thesis

Development of novel Quantum Algorithms for Near-term Quantum Devices for Chemical and Physical Problem Cases

Motivation:

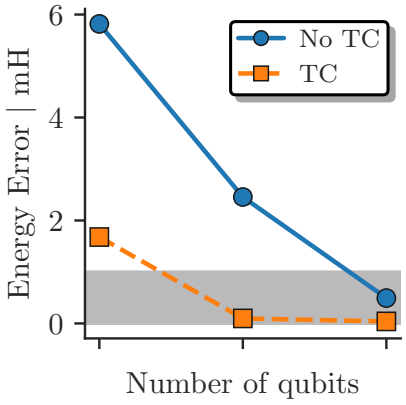
The calculation of ground state energies of molecules is expected to be one of the first practical applications of near-term quantum computers. Some of the advantage that a quantum computer offers, when applied to computational physics and chemistry, comes from an efficient representation of a quantum mechanical wavefunction on a quantum computer. This is achieved by using *quantum bits* (qubits) instead of ordinary bits as the basic unit of information and computation.



Current quantum hardware is however severely limited in the number of qubits and thus "state-of-the-art" calculations are only possible for very small problem cases. In our lab, we are developing a method to allow more accurate calculations requiring less quantum resources/qubits by incorporating part of the electronic correlation into the description of the problem at hand[1] and thus extending the applicability of current quantum computers to more realistic and interesting problem cases.

Project Description:

The goal of this master's thesis is to take part in the development of this so-called "transcorrelated (TC) method" and using it to perform highly accurate calculations in the field of computational chemistry and physics.



The initial part of the project will be focused on getting to know the field of quantum computational quantum chemistry and physics through study of published literature, such as [2], as well as getting acquainted with the tools used in the field (primarily IBM's open-source QISKit software solution will be used for this project [3]).

The second part of the project will focus on performing calculations using the transcorrelated method in conjunction with the Quantum Imaginary Time Evolution algorithm[4], first by simulation of a quantum device and subsequently by performing real experiments on quantum hardware provided by Chalmers and IBM.

As this work will be performed in collaboration with our industry partner, IBM Research Zürich, a stretch goal of this project is an incorporation of this method directly into QISKit. For this reason, upon available travel funds from Chalmers, research visits to the group of Dr. Ivano Tavernelli at IBM Research Zürich are a possibility.

Prerequisites:

a. Course in quantum mechanics and/or quantum information.
b. Coding experience in Python or a similar language (C++ or Fortran is an advantage)
c. Courses in physical chemistry and/or computational chemistry/physics, can be useful but are not mandatory.

Supervisors:

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References:

[1] Sokolov *et al*, arXiv preprint arXiv:2201.03049, (2022) [2] Bauer *et al.*, Chem. Rev. 120(22), 12685 (2020) [3] Aleksandrowicz, *et al*., *Qiskit: An Open-Source Framework for Quantum Computing* (Zenodo, 2019). [4] McArdle *et al. npj Quantum Inf* **5,** 75 (2019)