MINI-SCHOOL

NITheCS
National Institute for Theoretical and Computational Sciences

From Electrons to Qubits: Exploring the Frontiers of Electronic Structure

Shane McFarthing (Stellenbosch University)

Attend online: Wed 6, 13, 20 & 27 November 2024 @ 14h00-15h00 SAST

Understanding the electronic structure of molecules and other chemical systems is crucial for predicting chemical reactions, designing new materials, and advancing quantum chemistry in general. Classical approaches, such as Hartree -Fock (HF), Density Functional Theory (DFT), and Coupled Cluster (CC), have been widely used for solving the electronic Schrödinger equation, however they often suffer from limitations in their computational scaling or ability to effectively capture correlation effects.

A large focus in quantum computing is the revolution of this field by offering new algorithms that could overcome the computational limits of classical methods. The Variational Quantum Eigensolver (VQE), along with other quantum algorithms for ground-state energy estimation, aims to achieve more efficient solutions by combining classical optimization with quantum subroutines.

This Mini-school will guide participants through the foundational concepts of electronic structure theory, from traditional classical methods to state-of-the-art quantum and classical algorithms. Attendees will explore the advantages and limitations of both classical and quantum approaches, gain an understanding of key computational techniques, and develop insights into the future potential of quantum algorithms for large-scale systems.

COURSE PREREQUISITES: participants should have a basic understanding of quantum mechanics (undergraduate level) a basic knowledge of quantum computing, and basic linear algebra (undergraduate level).

LECTURE 1 (6 Nov 2024)

Introduction to Electronic Structure

This lecture will introduce the fundamental principles of electronic structure theory, focusing on the Schrödinger equation and its role in understanding the behaviour of electrons in molecules and materials. We'll also explore the practical applications of electronic structure methods in chemistry, materials science, and drug design.

LECTURE 2 (13 Nov 2024)

Classical Solutions – FCI and SCI

We'll dive into classical computing methods for solving electronic structure problems, starting with Full Configuration Interaction (FCI) for exact solutions before moving to conventional methods such as Hartree-Fock (HF) and Coupled Cluster (CC) theory. Lastly, we'll look at Selected Configuration Interaction (SCI) as an efficient alternative. Key advantages and limitations of these methods, such as scaling issues, will be discussed.

LECTURE 3 (20 Nov 2024)

Variational Quantum Eigensolver (VQE)

This lecture will introduce the Variational Quantum Eigensolver (VQE), a hybrid quantum-classical algorithm used to approximate ground states on quantum computers. We'll cover the set-up of the electronic structure problem on a quantum computer, ansatz construction, measurement strategies, and the strengths and challenges of VQE, particularly in handling noisy quantum hardware.

LECTURE 4 (27 Nov 2024)

State-of-the-Art Quantum Algorithms for Ground States

In this last session, we will explore cutting-edge quantum algorithms like ADAPT-VQE, and other emerging techniques. We'll compare these methods with the traditional approaches, discussing their potential to overcome current limitations and their prospects for future applications in electronic structure problems.

BIOGRAPHY

Shane studied Computer Science at the University of KwaZulu-Natal (UKZN) and completed his Masters in the study of variational quantum classifiers. He is currently a 2nd year PhD student in Physics at Stellenbosch University under the supervision of Prof F. Petruccione and Prof I. Sinayskiy, focusing on Noisy Intermediate-Scale Quantum (NISQ) algorithms, specifically efficient algorithms for the ground state search of chemical systems.

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