UNIVERSITÀ
DI TRENTO
Dipartimento di
Fisica

Dott.ssa Chiara Capecci

Università dell’Aquila

Wednesday, 19 July 2023: 11 a.m.
Room A209, Povo 1

Quantum Chemistry with Compact Circuits and Pulse-Based Ansatzes on NISQ devices

Abstract

Variational quantum algorithms offer a promising approach for studying quantum chemistry on noisy quantum computers. However, noise such as decoherence and unitary errors, imposes limitations on the depth of quantum circuits that can be effectively executed on hardware. This work aims to design compact and shallow parameterized circuit ansatzes that can capture the complexity of electronic structure problems. Two approaches are considered: one focuses on the development of improved Variational Quantum Eigensolver (VQE) algorithms using gate-based ansatzes and the other explores pulse-based optimization algorithms.

Modified VQE schemes are introduced to improve the wave function of the studied systems through the application of operators that allow a wave function expansion without a circuit ansatz extension. The non-unitary VQE (nu-VQE) method introduces a non-unitary operator called the Jastrow operator, inspired by classical Quantum Monte Carlo techniques.

The Wavefunction Adapted Hamiltonian Through Orbital Rotation (WAHTOR) algorithm leverages the invariance of the molecular Hamiltonian under orbital rotations to adapt the Hamiltonian coefficients to a given circuit ansatz. The algorithm's efficiency is demonstrated by testing different optimization procedures and showing the WAHTOR algorithm convergence to a specific basis set. Both methods, applied to prototypical molecular Hamiltonians, yield accurate variational energies with significantly reduced circuit depth.

Alternatively, encoding variational parameters directly as hardware pulse amplitudes and durations allows for further reduction in pulse schedules and overall circuit duration. This mitigates the impact of qubit decoherence and gate noise, enabling the study of larger and more complex molecular systems with higher precision. Applying the pulse-based variational algorithm (Pulse-VQE) to ground state computation of hydrogen-based systems using IBM cross-resonance hardware demonstrates a reduction in schedule duration of up to 5x compared to CNOT-based Ansatze, while also improving the measured energy.

Funded by the European Union under Horizon Europe Programme – Grant Agreement 101080086 — NeQST. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the granting authority can be held responsible for them.

NeQST