# QUANTUM COMPUTING FOR QUANTUM CHEMISTRY - REVIEW UCC METHODS AND ADAPT-VQE ALGORITHMS

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**Summary**

The use of quantum computers is a promising strategy to overcome challenges occurring in the area of quantum chemistry [1], [6]. Hardware quantum computers are supposed to potentially facilitate the encoding of the full configuration interaction (FCI) wavefunction of the many-electron molecular system thanks to entangled quantum bits or qubits. In classical computers, implementing the FCI scales exponentially with the number of electrons and the number of spin-orbitals, which makes the manipulation and storage of the wavefunction inefficient. However, using a quantum computer, we can instead store the (FCI) wavefunction by using only orbitals which corresponds to number of qubits. This potential quantum advantage has recently excited both hardware and software communities generating rapid progresses in the field. Variational Quantum Eigen solver (VQE) [5] is a potential algorithm-well suited for its practical implementation on present Noisy Intermediate Scaled Quantum (NISQ) devices.

The proposal presentation focuses on the development of Variational Quantum Eigensolvers (VQE) through an opensoure OpenVQE [4] , covering the latest advancements, circuit measurement techniques, and the computational demands of quantum computers. The process of VQE is hybrid, consists of quantum circuits state and classical parameter optimization, and it aims to find the ground state of a given molecular Hamiltonian [3]. Particularly, we will concentrate on advanced quantum chemistry methods such as Unitary Coupled Cluster that involves Single and Double excitations (UCCSD) has recently attracted interest due to its use in VQE molecular simulations on NISQ devices (recent reviews in [2]. Furthermore, we want to introduce, an algorithm termed Adaptive Derivative-Assembled Pseudo-Trotter (ADAPT)-VQE to build system-adapted ansatze with substantially fewer variational parameters. This section of the talk will introduce and compare two similar dynamically created ansatze(fermionic-ADAPT-VQE and qubit-ADAPT-VQE), and compare computational efficiency of ADAPT-VQE against UCCSD-VQE.

Through technical illustrations, we will demonstrate the differences in resource requirements between UCC and ADAPT-VQE, explained in a simple way. Attendees, including students and researchers, will explore the practical applications of both methods using the Quantum Learning Machine (QLM) and OpenVQE—tools designed specifically for quantum chemistry simulations. Participants will gain valuable insights into the construction of ansätze, learning to distinguish between iterative and non-iterative approaches

## References


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