Computational Complexity of UCC Ansatz in VQE

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The development in our ability to control quantum systems over the last few decades has significantly increased interest in second-generation quantum technologies and raised numerous questions about their applications in various fields. Specifically, highly precise control over quantum systems can be used to simulate other quantum systems, a process known as quantum simulation. Quantum simulations are particularly necessary due to the challenges of preparing and measuring the properties of scientifically significant quantum systems, such as molecular properties and dynamics in chemistry.

One of the most prominent algorithms in the noisy intermediate-scale quantum (NISQ) era aimed at obtaining information about molecules is the Variational Quantum Eigensolver (VQE). This algorithm involves constructing a parameterized quantum system that transitions an initial quantum state to the ground state of a given Hamiltonian by optimizing the parameters using a classical optimizer. Despite the potential quantum advantages of this algorithm, a thorough study of its complexity is required. This involves examining which methods can be applied at each stage, how they can be combined, and what quantum hardware they can be implemented on.

In this study, we focus on the complexity of the quantum circuit, or ansatz. We analyzed the Unitary Coupled Cluster (UCC) ansatz and its variants. This ansatz is based on the Coupled Cluster theory, one of the most successful theories for simulating molecules using classical computers. Our investigation covers the types and quantities of operations needed to implement the ansatz, how these operations scale with system size, and how to reduce them.