CP-05-02

Current status of variational quantum algorithms for chemistry and beyond

Wataru Mizukami

Center for Quantum Information and Quantum Biology, Osaka Univ., Japan

Abstract

Quantum chemistry has been seen as a promising application for quantum computers so far. Driven by this expectation, the development of algorithms for quantum chemistry using quantum computers has been active over the past five years. As a result, variational quantum algorithms (VQAs) can now be used to perform a wide range of chemical calculations with quantum circuit emulators. Such state-of-the-art VQAs have been implemented in various open-source software and cloud services and are readily available to anyone. On the other hand, the challenges for the practical application of quantum chemical calculations using real quantum computers are becoming increasingly clearer. In this talk, I will first introduce our progress in quantum chemical calculations using VQA. Next, I will introduce 1) our recently-proposed perturbation theory using quantum signal processing [arXiv:2210.00718] and 2) resource estimation for phase estimation for model Hamiltonians [arXiv:2210.14109], respectively, and discuss challenges that lie ahead.