Title: Variational quantum computation of linear response properties of molecules on a superconducting quantum processor

Wei-Hai Fang
Beijing Normal University, Beijing 100875, China

Abstract

Predictive simulation of molecular response properties such as electronic absorption spectra is of great technological importance, but remains a long-standing computational challenge for electronic structure methods on classical computers. While quantum computers hold the promise to solve this problem more efficiently in the long run, existing quantum algorithms requiring deep quantum circuits are infeasible for near-term noisy quantum processors. Here, we report the variational quantum computation of linear optical properties of molecules on a superconducting quantum processor enabled by a hybrid quantum-classical approach. We demonstrate the feasibility of this approach for computing dynamic polarizabilities of the hydrogen molecule, and then apply it to tackle two representative problems of practical significance, including simulating ultraviolet-visible absorption spectra of polyacenes and X-ray absorption spectra of carbon monoxide.