Non-adiabatic Molecular Dynamics on Quantum Computers

Yu Zhang

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545
Email: zhy@lanl.gov

Non-adiabatic molecular dynamics is essential for understanding the excited state phenomena. The major bottleneck of quantum molecular dynamics is the calculations of electronic states, their derivatives, and derivative couplings between different excited states. Hence, extensive efforts have been recently made to leverage quantum computers to revolutionize the computational of electronic states. The variational quantum eigensolver (VQE) is the most widely used algorithm nowadays. However, the VQE-type methods suffer from optimization problems, and most of the current VQE algorithms only focus on the ground state. To overcome these obstacles, we developed an efficient quantum Krylov subspace algorithm by leveraging the iterative growth of the Krylov subspace. Such subspace methods remove the optimization problems suffered in the VQE-type of methods. The newly proposed quantum Krylov subspace algorithm is employed to study the excited-state properties of various systems on both simulators and quantum devices. In addition, we developed a framework to measure the non-adiabatic couplings between different electronic states on quantum computers. Consequently, a hybrid quantum-classical algorithm for non-adiabatic molecular dynamics is developed. We believe that our recent developments provide a feasible tool for studying excited-state and non-adiabatic phenomena on quantum computers.