Contribution ID: **128** Type: **Poster**

Shorcuts for Adiabatic and Variational Algorithms in Quantum Chemistry

Quantum computation has sparked a revolution in solving problems ranging from combinatorial optimization or quantum chemistry to industrial applications. Numerous algorithm proposals have emerged in recent years, including adiabatic and variational quantum algorithms, which have shown promising results in current NISQ devices. To further reduce the quantum resources required, digitalized counter-diabatic quantum algorithms have been proposed.
Our work focuses on designing a counter-diabatic term for adiabatic and variational quantum algorithms in the quantum chemistry framework. By incorporating the counter-diabatic term, we were able to calculate the ground state of a set of molecules with great convergence in both adiabatic and VQE algorithms. We also proposed a new ansatz, the Adiabatic Gauge Ansatz (AGA), based on the adiabatic gauge potential for VQE, which demonstrated good convergence with a reduced number of terms, even considering only up to two-body interactions.
Our implementation of the counter-diabatic term in the adiabatic algorithm demonstrates a substantial improvement in computation speed and a reduction of the Trotter error. Additionally, in the variational algorithm, we found that our approach achieves comparable accuracy to the widely used UCCSD ansatz while significantly reducing quantum resources, particularly in the proximity of the bond distance.

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