Quantum Imaginary Time Evolution for Ground and Excited States

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Advances in quantum information and technology have recently attracted widespread interest in various fields in the hope to overcome the limitations that the current digital computers are facing. Quantum chemistry is one such area and is believed to become a killer application for quantum computing.

In this talk, I will introduce some of our recent efforts on developing new quantum algorithms that are combined with classical simulations, aiming for proper descriptions of strongly correlated systems and their excited states. I will first provide a more robust derivation of quantum imaginary time evolution (QITE) proposed by Motta et al. in 2020. The improved algorithm allows for a better unitary approximation of imaginary time propagation, and thus much faster convergence of ground state with respect to imaginary time β using a quantum computer. Since the equation is correct to second order of imaginary time step $\Delta\beta$, the performance of our algorithm is almost independent of the choice of $\Delta\beta$, which is not the case for the original QITE algorithm. Then, I will discuss how one can tackle excited states by extending QITE. The first approach is based on the propagation of $(\hat{H}-\omega)^2$ to target the excited state that has the energy closest to ω. The second approach treats a model configuration space that is comprised of multiple states, and propagates it to the exact space. I will compare the two methods using numerical simulations and discuss their advantages and disadvantages.