# Quantum Algorithm for Optimal Molecular Geometries Based on Probabilistic Imaginary-Time Evolution

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The widely adopted approach for computations using quantum computers is currently the variational algorithm, which involves optimizing parameters characterizing quantum circuits using classical computers. Various improvements and extensions have been proposed for such circuits (variational circuits), but fundamentally, they can only optimize quantum states within the scope anticipated by variational circuits.
On the other hand, we have recently introduced a general non-variational algorithm, the Probabilistic Imaginary-Time Evolution (PITE), which does not rely on the concurrent use of classical computers [Kosugi et al., Phys. Rev. Research 4, 033121 (2022)].
Unlike the variational algorithm, one of the distinguishing features of PITE is its ability to perform true quantum optimization. This characteristic is particularly pronounced in quantum chemistry calculations in the first quantization formalism.
In this presentation, we extensively elaborated on the scalability of computations in both classical preprocessing and subsequent quantum calculations from the perspective of first quantization formalism.
Furthermore, by introducing registers for encoding nuclear configurations, we recently discovered the capability of using PITE for molecular structure optimization. We introduced a novel method based on this approach and demonstrated that achieving quantum advantage is possible for both electronic and nuclear degrees of freedom.