Geometric optimization based on first-quantized Hamiltonian using imaginary-time evolution on a quantum computer

Yu-ichiro Matsushita

Quantum computers are considered promising alternatives to classical computers due to their high expressive power in encoding the spatial distribution of wave functions. In our research group, we propose the imaginary time evolution method as a non-variational approach for calculating the ground state in many-body problems. In this study, we have developed a quantum algorithm for the structural optimization of molecules based on the first quantized Hamiltonian, utilizing the imaginary time evolution method. In the proposed framework, atomic nuclei are treated as classical point charges, while electrons are treated as quantum-mechanical particles. This corresponds to an exhaustive exploration of countless geometric candidate structures. Moreover, encoding atomic nuclei classically eliminates the need to represent wave functions on the femtometer scale, reducing the required number of qubits.

By iteratively measuring the output states generated through the imaginary time evolution, we obtain a histogram that provides the global minimum energy landscape. We expect that the method proposed in this study will contribute to the realization of practical quantum computers in quantum chemistry.