Imaginary-time evolution with a single ancilla: first-quantized eigensolver for electronic structure calculation in quantum chemistry

Quantum computation algorithms for obtaining the ground state of a given Hamiltonian are in strong demand, for example in quantum chemical calculations and optimization. In this study, we propose a new ground-state computation framework based on the imaginary-time evolution method for error-tolerant quantum gated computers.

Due to the non-unitary nature of the imaginary-time evolution method, its implementation in quantum circuits is not simple. However, we proposed a method that makes this possible by extending the space by adding an auxiliary bit and by using the observation of the auxiliary bit, and named it the probabilistic imaginary-time evolution (PITE) method. Specifically, the circuit is configured so that if an auxiliary bit is observed and a zero state is obtained with a certain probability, an imaginary-time evolved quantum register state is obtained. This differs significantly from existing methods in that it is non-variational. In addition, PITE circuits can be constructed if real-time evolution with a given Hamiltonian can be implemented, and many existing techniques for real-time evolution can be applied without modification.

Furthermore, as an example of the application of PITE to quantum chemical calculations, a scheme based on first quantization is proposed and named First-quantum Eigensolver (FQE). In terms of the number of operations, the first-quantum Eigensolver shows better scaling with respect to the system size than the second-quantum Eigensolver.

Based on the PITE method, structural optimization of molecular systems, application to calculations of systems under magnetic fields, and combination with quantum amplitude amplification have already been reported from our group, showing the wide applicability of the PITE method.