Toward large-scale quantum chemical calculations with annealers: Divide-and-conquer (DC) and annealing + Bayesian-optimization configuration interaction (ABCI) methods

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One of the goals of quantum chemistry is to accurately solve the Schrödinger equation for realistic systems. However, even mean-field Hartree-Fock or DFT calculations require diagonalization of the one-electron Hamiltonian matrix, which requires a computational time proportional to at least $O(N^3)$ for N atomic system. Furthermore, the scaling rapidly increases as the accuracy of the adopted wave function theory improves. In addition, as the speed of classical Neumann-type computers is getting saturated, the development of electron correlation theory that accurately solves the Schrödinger equation using novel-conceptual computers (quantum computers, classical annealing computers, etc.) has attracted significant attention.

We have developed an $O(N)$ quantum chemical calculation method called the divide-and-conquer (DC) method [1], which was originally proposed by Yang and coworkers [2]. In the first half of this presentation, we will first review our recent developments in the DC methods; especially focusing on the automatic determination of the buffer region [2-4], which affects both the accuracy and computational time of the DC calculations, and the semi-empirical DC method.

The Xia-Bian-Kais (XBK) transformation [5,6], which maps the second quantized Hamiltonian into the Ising Hamiltonian, is a method for optimizing the CI wavefunction using an annealing computer. In the latter half, we propose a method named the annealing + Bayesian-optimization configuration interaction (ABCI) method to reduce the number of qubits used in the XBK transformation by introducing weight bits that are determined by the Bayesian optimization.

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