Noisy simulations of first-principles calculations using quantum classical hybrid algorithms

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In recent years, quantum computers with dozens of qubits have been built; we now expect to see quantum devices with hundreds of qubits in the near future. Such quantum computers are often called noisy-intermediate scale quantum devices (NISQs) since they do not have quantum error correction functionality. Nonetheless, in 2019, Google showed that a NISQ with as few as 53 qubits could already outperform supercomputers when limited to a specific task. Many research projects have been currently underway to exploit the computational potential of NISQs.

One promising algorithm for NISQs is the quantum-classical hybrid algorithm, which can operate even in the short coherence time of a NISQ. Among them, the variational quantum eigensolver (VQE) can be applied to first-principles calculations of materials or molecules. An advantage of the VQE is that it can parametrize some wave functions ansatzes such as unitary coupled clusters (UCC)in polynomial time, while the UCC is exponentially computationally expensive on classical computers. However, if a NISQ is used for the VQE, the computational results are unavoidably affected by noises.

In this work, we have investigated the influence of this noise on the VQE by using a quantum circuit simulator. There are many types of noises in quantum computers, such as read-out error and amplitude damping. Since it is difficult to model all kinds of errors, we have only dealt with depolarizing noise, which is a typical error model for quantum computers, in this study. This noise can be described as Pauli operators probabilistically acting on each gate of a quantum circuit. In the presence of depolarizing noise, we can effectively say that the noise probabilistically changes the quantum circuit at each sampling. It means that the numerical simulations with depolarizing noise using classical computers, are required to simulate various quantum circuits: the simulation with depolarizing noise is much more expensive than the simulation without it. Besides, because such a simulation is a sampling problem, the individual circuits changed by the noise are independent. Hence, the VQE with depolarizing noise can be highly parallelizable.

This year, we have realized the simulation with depolarizing noise up to 1 million samples

by using the MPI parallelization and the supercomputer of the ISSP. In addition, by using a many-body expansion, we have studied the effect of depolarizing errors on up-to a 100-qubits problem. We have chosen the most basic molecule, the hydrogen molecule, as the benchmark system. In our program, the PySCF quantum chemistry program library [1] is used to prepare the second quantized electronic Hamiltonian; Qulacs is employed as a quantum circuit simulator [2]. The obtained numerical results illustrate that it is impractical to achieve chemical accuracy with the error rates of today's quantum computers. This implies that an efficient way to suppress the effect of depolarizing noise is vital for the practical application of first-principles calculations using NISQs.

References

[1] Q. Sun et al., WIREs Comput. Mol. Sci. **8**, e1340 (2017).

[2] Y. Suzuki et al., arXiv:2011.13524