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Implementation of imaginary-time evolution method on a quantum computer and its applications to quantum chemical calculations

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Abstract

In 2019, Google reported quantum supremacy in a gated quantum computer, and there has been a growing interest in quantum computing since then. In particular, quantum chemical computation is a field where quantum computers are expected to be utilized at an early stage, and many researchers are participating in the development of its algorithms. In recent years, research on the Variational Quantum Eigensolver (VQE) based on the variational principle as a method for quantum chemical calculations on noisy intermediate-scale quantum (NISQ) devices, which are small-to-medium scale quantum computers, has been actively conducted all over the world. However, many problems have been pointed out in VQE, and it is not clear whether VQE will be an effective application for quantum chemical calculations or not.

In contrast, we are developing algorithms for fault-tolerant quantum computers that are not based on the variational principle and applying them to the field of quantum chemical calculations. In particular, we have developed an algorithm of "imaginary-time evolution" on a quantum computer, called Probabilistic Imaginary-Time Evolution (PITE) [1]. We have also succeeded in mathematically proving the quantum advantage of PITE in solving problems faster than classical computers[2][3][4]. In this presentation, I will discuss the difference between a quantum computer and a classical computer, the quantum algorithm we are developing, i.e., PITE, and differences between PITE and other algorithms. I will also show some application results of PITE to quantum chemical calculations[5].

References
[1] Phys. Rev. Research **4** (2022)033121. [2] Phys. Rev. Research **5** (2023)043048.
[3] arXiv:2308.03605 (2023). [4] arXiv:2212.13816(2022).
[5] arXiv:2210.09883(2022), accepted in npj Quantum Inofrmation (2023).