Accelerating ground state calculation using probabilistic imaginary-time evolution and quantum amplitude amplification

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In the rapidly advancing field of quantum computing, numerous studies are being conducted. Particularly, the preparation of the ground state of many-body problems in the realm of materials science has become a critical challenge. Ground state calculations are exceedingly vital in investigating the properties of various materials. Recently, we've turned our attention to the Probabilistic Imaginary-Time Evolution (PITE) method, a non-variational approach to ground state calculations [1]. This method combines auxiliary bits and measurements to achieve non-unitary imaginary-time evolution operators on quantum computers. However, due to the probabilistic nature of PITE, the success probability throughout all imaginary time steps had limitations.

To address this drawback, we introduce a combination of Quantum Amplitude Amplification (QAA) with PITE to overcome this limitation. Furthermore, based on an analysis of the computational resources of PITE, it was discovered that its probabilistic nature was a source of computational performance degradation [2]. The QAA method is proposed as a solution to this constrained computational performance, leading to a quadratic speedup of the PITE method [3,4].

Insights from this research are likely to contribute to future studies of ground state calculations on quantum computers.

Reference:

[1] T. Kosugi, Y. Nishiya, H. Nishi, and Y.-i. Matsushita, Phys. Rev. Res. 4, 033121 (2022).

[2] H. Nishi, K. Hamada, Y. Nishiya, T. Kosugi, and Y.-i. Matsushita, arXiv:2305.04600 (2023).

[3] H. Nishi, T. Kosugi, Y. Nishiya, Y.-i. Matsushita, arXiv:2212.13816 (2022).

[4] H. Nishi, T. Kosugi, Y. Nishiya, Y.-i. Matsushita, arXiv:2308.03605 (2023).