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Title; Deep variational quantum eigensolver (Deep VQE) for low-energy eigenstates

Abstract;

Quantum computation has become one of the most intriguing fields in today's science. In particular, Noisy-Intermediate Scale Quantum (NISQ) devices, which are quantum computers having O(100)-O(1000) qubits without fault-tolerance, have experienced a rapid growth due to their near-term applications. Variational Quantum Eigensolver (VQE) is one of the most promising algorithms which work on NISQ devices.

VQE is a quantum-classical hybrid algorithm for simulating low-energy eigenstates of quantum many-body systems, which usually requires much memory and much time under classical computation. However, VQE requires NISQ devices as large as quantum systems we want to simulate, and the size of today's NISQ devices is not sufficient for tackling practical problems in condensed matter physics and quantum chemistry. Thus, it is necessary to construct algorithms that can simulate large quantum systems with small NISQ devices.

Here, we construct a quantum-classical hybrid algorithm dubbed "Deep VQE", which combines VQE with coarse-graining [1,2]. In Deep VQE, we repeat VQE and coarse-graining with choosing local excitations relevant for ground states. Due to the efficient representation of ground states by coarse-graining, Deep VQE can compute approximate ground states of large quantum systems with smaller NISQ devices [1]. Furthermore, we extend Deep VQE to compute low-energy excited eigenstates by elaborating coarse-graining, and numerically verify the applicability of our algorithm to spin systems and periodic materials with reducing the size of NISQ devices [2]. These results will lead to acceleration in the application of NISQ devices to condensed matter physics and quantum chemistry.

References;

[1] K. Fujii, K. Mitarai, W. Mizukami, and Y. O. Nakagawa, arXiv 2007.10917 (2020)

[2] K. Mizuta, M. Fujii, S. Fujii, K. Ichikawa, Y. Okuno, Y. O. Nakagawa. arXiv:2104.00855 (2021)