Accelerated variational quantum eigensolver with joint Bell measurement

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The variational quantum eigensolver (VQE) stands as a prominent quantum-classical hybrid algorithm for near-term quantum computers to obtain the ground states of molecular Hamiltonians in quantum chemistry. However, due to the non-commutativity of the Pauli operators in the Hamiltonian, the number of measurements required on quantum computers increases significantly as the system size grows, which may hinder practical applications of VQE. In this work, we present a protocol termed *joint Bell measurement VQE* (JBM-VQE)(a schematic illustration is provided in Fig. 1) to reduce the number of measurements and speed up the VQE algorithm. Our method employs joint Bell measurements, enabling the simultaneous measurement of the absolute values of all expectation values of Pauli operators present in the Hamiltonian. In the course of the optimization, JBM-VQE estimates the absolute values of the expectation values of the Pauli operators for each iteration by the joint Bell measurement, while the signs of them are measured less frequently by the conventional method to measure the expectation values. Our approach is based on the empirical observation that the signs do not often change during optimization. We illustrate the speed-up of JBM-VQE compared to conventional VQE by numerical simulations for finding the ground states of molecular Hamiltonians of small molecules, and the speed-up of JBM-VQE at the early stage of the optimization becomes increasingly pronounced in larger systems. Our approach based on the joint Bell measurement is not limited to VQE and can be utilized in various quantum algorithms whose cost functions are expectation values of many Pauli operators.

The extended manuscript of this abstract can be accessed at Ref. [1].

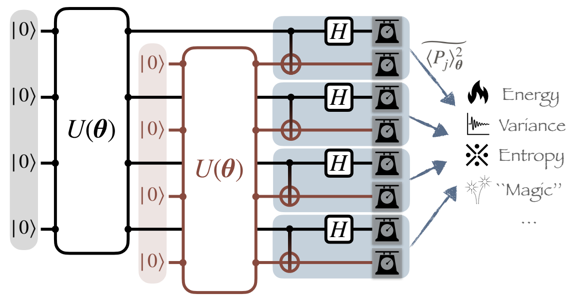

Figure 1. Schematic picture of the joint Bell measurement and JBM-VQE. For an n-qubit quantum state $|\psi(\boldsymbol{\theta})\rangle = U(\boldsymbol{\theta})\,|0\rangle$, the $2n$-qubit quantum states $|\psi(\boldsymbol{\theta})\rangle \otimes |\psi(\boldsymbol{\theta})\rangle$ is prepared and measured in the Bell basis. The measurement results can give the estimates of all expectation values $\langle P_j \rangle_{\boldsymbol{\theta}}^2 = (\langle \psi(\boldsymbol{\theta})|P_j|\psi(\boldsymbol{\theta})\rangle)^2$ in the original n-qubit systems, and the state information (energy in JBM-VQE) is estimated by these estimates as well as the pre-given signs of the expectation values.

[1] C. Cao, H. Yano, and Y. O. Nakagawa, Accelerated variational quantum eigensolver with joint bell measurement, Phys. Rev. Res. **6**, 013205 (2024).

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