Supplementary material for: Variational quantum eigensolver with mutual variance-Hamiltonian optimization

Bin-Lin Chen(陈彬琳)¹, Dan-Bo Zhang(张旦波)^{2,1*}

¹Guangdong Provincial Key Laboratory of Quantum Engineering and Quantum Materials,

School of Physics and Telecommunication Engineering,

South China Normal University, Guangzhou 510006, China

²Guangdong-Hong Kong Joint Laboratory of Quantum Matter,

Frontier Research Institute for Physics, South China Normal University, Guangzhou 510006, China

The hybrid quantum-classical optimization for minimizing the cost function at the wavefunctionsearching stage requires to calculate gradients of the energy variance. However, the optimization can be difficulty due to barren plateaus, which states that the gradients can vanish exponentially with the increasing of qubit number or circuit depth for general random circuits such as the hardware efficient ansatz^[1]. The issue of barren plateaus is related both to the type of cost function [2] as well as the architecture of parameterized quantum circuits ^[3]. In this paper, we adopt energy variance instead of energy in the cost function. Moreover, the ansatz inspired by the Hamiltonian variational ansatz (HVA), called as multi-angle HVA, is designed specifically for solving the fully-connected Ising model. In this regard, it is necessary to explore whether the issue of barren plateaus still exist.

For this, we compare variances of gradients for cost function of both energy and energy variance under the multi-angle HVA (Fig. s1 (a)) and the hardware efficient ansatz (Fig. s1 (b)), respectively. The hardware efficient ansatz is universal, whose each block consisted two layers of one-qubit rotations and one layer two-qubit entangled gates. The gradients at larger size and deeper depth are calculated. A random sampling method is adopted to evaluate the variance of gradients, where one tenth of the total number of input parameters is randomly sampled each time and the sampling is repeated 20 times. As seen in Fig. s1, variances of gradients under both ansatzs and for both energy and energy variance decrease exponentially with the increasing of qubits. This indicates that the multi-angle HVA in our paper share the same issue of barren plateaus as the hardware efficient ansatz. To solve the barren plateaus problem, one should refer to more specific ansatz. In addition, it is observed in Fig. s1 (a) that the vanishing of gradients with the circuit depth is not obvious for both energy and energy variance, which indicates that the multi-angle HVA may reduce the vanishing of gradients for deep quantum circuit.



Fig. s1. Variance of gradients evaluated by random sampling for both VQE(solid line) and HG-VVQE(dashed line). The fully connected transverse-field Ising model is adopted. (a) The multi-angle Hamiltonian variational ansatz used in the paper. (b) Hardware efficient ansatz.

参考文献

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^{*}Corresponding authors. Email: dbzhang@m.scnu.edu.cn