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# Purified subspace-search variational quantum eigensolver

Variational quantum algorithms (VQA) are mainly designed to obtain an approximation for the ground state of a target Hamiltonian. Methods based on VQA for calculating excited states currently involve high-depth unitary implementation or state-specific optimizations on top of previously-found ground states. To directly extend the VQA framework to excited states, we propose an algorithm based on our recent purification of weighted ensemble states [1]. This algorithm uses the Gross-Oliveira-Kohn variational principle used in excited-state density functional theories and chooses the appropriate set of weights to construct a Bardeen-Cooper-Schrieffer (BCS)-like state in a well-defined duplicated Hilbert space. The exponential form of such a BCS-like state allows a quite efficient implementation of a VQA for excited states on near-term quantum devices. Combining a variational quantum circuit and a neural network, our algorithm can obtain, for finite Hamiltonians, all the excited states we want.

[1] C. L. Benavides-Riveros et al., Phys. Rev. Lett. 129, 066401 (2022).

## Abstract category

Quantum Computing

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