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A device-oriented optimizer for solving ground state problems on an approximate quantum computer, Part I: Theory ANTONIO MEZZACAPO, ABHINAV KANDALA, KRISTAN TEMME, SERGEY BRAVYI, MAIKA TAKITA, JOSE CHAVEZ-GARCIA, ANTONIO CÓRCOLES, JOHN SMOLIN , JERRY CHOW, JAY GAMBETTA, IBM T. J. Watson Research Center — Quantum-classical variational eigensolvers provide a method to solve for ground state of Hamiltonian problems. Their performance has been recently investigated for interacting fermionic problems, which are believed to be suitable bench tests for medium-sized quantum computers. The overhead cost in terms of computational time, size and quality of the actual available quantum hardware is therefore crucial. In this talk we first present methods to reduce the number of qubits required to encode fermionic problems. We then discuss how the efficiency of the quantum part of the optimization problem can be increased by a device-oriented design of the state preparation. We present a numerical study of the method for generic fermionic problems of increasing size, including molecular structure ones.

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