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A Hybrid Classical/Quantum Approach for Large-Scale Studies of Quantum Systems with Density Matrix Embedding Theory NICHOLAS RUBIN¹, Rigetti Quantum Computing — Determining ground state energies of quantum systems by hybrid classical/quantum methods has emerged as a promising candidate application for near-term quantum computational resources. Short of large-scale fault-tolerant quantum computers, small-scale devices can be leveraged with current computational techniques to identify important subspaces of relatively large Hamiltonians. Inspired by the work that described the merging of dynamical mean-field theory (DMFT) with a small-scale quantum computational resource as an impurity solver [Bauer et al., arXiv:1510.03859v2], we describe an alternative embedding scheme, density matrix embedding theory (DMET), that naturally fits with the output from the variational quantum eigensolver and other hybrid approaches. This approach is validated using a quantum abstract machine simulator [Smith et al., arXiv:1608.03355] that reproduces the ground state energy of the Hubbard model converged to the infinite limit. We comment on the implementation of this algorithm in near-term superconducting processors.

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