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Anderson impurity solver integrating tensor network methods with quantum computing

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Solving the Anderson impurity model typically involves a two-step process, where one first calculates the ground state of the Hamiltonian, and then computes its dynamical properties to obtain the Green's function. Here we propose a hybrid classical/quantum algorithm where the first step is performed using a classical computer to obtain the tensor network ground state as well as its quantum circuit representation, and the second step is executed on the quantum computer to obtain the Green's function. Our algorithm exploits the efficiency of tensor networks for preparing ground states on classical computers, and takes advantage of quantum processors for the evaluation of the time evolution, which can become intractable on classical computers. We demonstrate the algorithm using 20 qubits on a quantum computing emulator for SrVO3 with a multi-orbital Anderson impurity model within the dynamical mean field theory. The tensor network based ground state quantum circuit preparation algorithm can also be performed for up to 40 qubits with our available computing resources, while the state vector emulation of the quantum algorithm for time evolution is beyond what is accessible with such resources. We show that, provided the tensor network calculation is able to accurately obtain the ground state energy, this scheme does not require a perfect reproduction of the ground state wave function on the quantum circuit to give an accurate Green's function. This hybrid approach may lead to quantum advantage in materials simulations where the ground state can be computed classically, but where the dynamical properties cannot.

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