The q-HEOM method: A quantum algorithm for simulations of open quantum system dynamics on quantum computers

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The hierarchical equations of motion (HEOM) method enables rigorous simulations of open quantum system dynamics. The effects of the harmonic bath that couples to the system are explained in terms of a reservoir correlation function which is decomposed into a sum of exponential functions of time. On classical computers, the computational cost grows exponentially with an increasing number of terms in the correlation function or increasing strength of the system-environment coupling. Quantum computing opens a new opportunity for more efficient simulations of open quantum system dynamics. Here, we introduce a simple quantum algorithm to implement the HEOM method on a quantum computer. The non-unitary propagator that describes the evolution of the subsystem density matrix with dissipation is dilated into a unitary propagator in a higher-dimensional Hilbert space with ancilla qubits. We demonstrate the capabilities of the resulting q-HEOM method as applied to simulations of model systems of chemical and biological interest, including benchmark calculations of energy transfer in the Fenna-Matthews-Olson (FMO) complex, and charge transfer in donor-acceptor spin-boson model systems.