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Resource estimates for the open-system simulation of chemical reactions

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Open quantum systems evolving under time-dependent Lindbladian simulations dynamics arise in diverse contexts, yet efficient algorithms for large-scale, time-dependent Lindbladian dynamics remain underexplored. In the fault-tolerant setting, the time required to propagate a state by a complex, time-dependent Hamiltonian is prohibitive. We circumvent this issue by introducing a discretization-and-thermalization framework for simulating such dynamics, followed by detailed numerical analysis and resource estimation for chemically reactive systems undergoing environment-influenced reaction pathways. The inclusion of T-gate and logical qubit counts offers practical guidance for future implementations, making this framework relevant to a broad range of applications, including fermionic, spin, and chemically reactive systems.

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