

Abstract Submitted
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Transition Path Sampling Rare Events In non-Markovian Open Quantum Systems¹ LEONEL VARVELO, DORAN BENNETT, Southern Methodist University — Rare events in excited state dynamics, such as transport across grain boundaries, are difficult to simulate due to large time scales and high computational expense of quantum dynamics algorithms. We present a new method for extending timescales of quantum simulations using transition path sampling. Implementing the Hierarchy of Pure States (HOPS) method, a formally exact equation of motion for open quantum systems, we construct independent stochastic trajectories which are used to produce a quantum path ensemble. Using transition path sampling we can directly construct a reactive ensemble, where each member of the ensemble is a realization of the rare event in a non-Markovian system. Combining quantum transition path sampling with the weighted histogram analysis method (WHAM) we can efficiently study the dynamics of rare events in non-Markovian systems within the formally exact HOPS equation-of-motion.

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