Efficient Simulation of Non-Markovian Open Systems Using Real Time Path Integrals

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Many methods of describing open quantum system dynamics rely on perturbative approaches. Accurately capturing strong coupling and the non-Markovian physics that accompanies it is extremely challenging and for consistently reliable results one must turn to numerical methods. One such method is the augmented density tensor method [1], based on the path integral approach, whose defining feature is the finite memory approximation, where non-Markovian correlations in the reduced system are given finite range by discarding long ranged bath correlations. Despite its successes, a major drawback is that for some bath spectral densities the scheme produces unphysical system states.

We identify the source of this unphysical system evolution in an exact independent boson model in which the memory cutoff is imposed on the solution. For non-Markovian environments in which transient negative decay rates occur the use of the finite memory approximation can result in eternal exponential growth of density matrix elements, making the state non-positive and unphysical. We thus propose an alternative way of making the finite memory approximation without discarding any bath correlations, in a way that guarantees that the augmented density tensor method reproduces the exact solution identically.

We put our method to use by studying the Spin-Boson model with a superohmic environment, over a range of parameters that would have been inaccessible previously, and find features in the dynamics which we argue to be information backflow from the environment to the system. Additionally, we show our new method can be used in fixing unphysical exponential growth in non-equilibrium correlation functions computed using the augmented density tensor method, with potential application in the calulation of emission and absorption spectra of quantum dots.

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