## Updated Quantum Master Equations for Simulation of Open Quantum Dynamics

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Predicting the dynamics of a quantum systems is a key task in quantum theory. Doing so for large Hilbert spaces, however, is impractical. A qubit coupled to a bosonic environment, for example, has infinite dimensions and thus keeping track of the dynamics of both system and bath is typically not possible. Alternatively, following the dynamics of the qubit is possible by tracing out the environment, leading to methods such as the quantum master equation [1]. In such open quantum system approaches, one only needs the correlations of the bath operators, which can be experimentally obtained by performing the quantum noise spectroscopy [2], in order to simulate the dynamics. However, this method is used together with the weak coupling, Gaussian correlation assumptions, or Born approximation, in order to limit the amount of required seed information about the environment. This usually implies that - barring particularly friendly models - the prediction is often only reliable for short times. In this work, we introduce a new method to simulate the dynamics of an open quantum system by using a hierarchy of master equations, which update not only the relevant information about the system but also the leading correlations of the bath operators. Our method takes into account the fact that the state of the bath evolves not only due to its own dynamics but also due to the coupling to the system, therefore it provides a more accurate description of the dynamics. We compare the performance of our method to the well-known Nakajima & Zwanzing master equation [3, 4], and show that by updating the correlations one can predict the dynamics of the system for longer time using the same seed information. We also show how we can accurately track the relevant bath correlations relative to the system-bath state at a given time. Our work paves the way to comprehensively describing and eventually controlling open quantum systems in the presence of quantum non-markovian environments.

[1] Breuer, H.-P. and Petruccione, F. The Theory of Open Quantum Systems (Oxford Univ. Press, 2002).

[2] T. Chalermpusitarak, B. Tonekaboni, Y. Wang, L. M. Norris, L. Viola, and G. A. Paz-Silva, *Frame-based filter function formalism for quantum characterization and Control*, PRX Quantum 2, 030315 (2021).

- [3] S. Nakajima, Prog. Theor. Phys. 20, 948 (1958).
- [4] R. Zwanzig, J. Chem. Phys. 33, 1338 (1960).