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A system-bath model to investigate the interaction of a molecule with its environment

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Addressing the dynamics of molecular systems coupled to an environment is a challenging task, especially when considering finite-size environments that can be affected by their interactions with the smaller system. In such cases, the usual open quantum system methods and approximations might fail as they assume that the environment (or "bath") is infinite, always at thermodynamical equilibrium, and not perturbed by the system [1]. In particular, they do not take into account the fact that finite environments can be heated by the excitation of the system and evolve out of equilibrium. For example, such situations may occur when studying molecules in clusters or matrices [2], or when probing small molecules trapped in fullerenes [3] or clathrates [4].

In this context, we are developing a new theoretical model based on a system-bath approach where we consider a one-dimensional system (*e.g.* one vibrational mode) interacting with a large harmonic bath (˜100-1000 modes). The system and its coupling to individual bath modes are treated as rigorously as possible but the bath part of the Hamiltonian is simplified with its modes being replaced by a ladder of effective quantum energy states which describes the energy stored in the bath. This model allows us to study the relaxation dynamics of the system at finite temperature and to analyze the response of the bath to the system's excitation. In this contribution, we will present the first results obtained by using this method on a system taken from [5], where an O-H stretching mode interacts with a "surface"modeled by a set of 40 to 800 harmonic oscillators.

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