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Quantum energy and coherence exchange with discrete baths

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HIGHLIGHTS

- Quantum coherence of systems coupled to finite baths composed of N harmonic oscillators is investigated.
- A stochastic Schrödinger equation is solved numerically.
- The energy and purity exchange between system and bath are described in details as a function of the numbers of bath harmonic oscillators.
- The non-Markovian dynamics due to finite baths is analyzed.

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ABSTRACT

Coherence and quantum average energy exchange are studied for a system particle as a function of the number N of constituents of a discrete bath model. The time evolution of the energy and coherence, determined via the system purity (proportional to the linear entropy of the quantum statistical ensemble), are obtained solving numerically the Schrödinger equation. A new simplified stochastic Schrödinger equation is derived which takes into account the discreteness of the bath. The environment (bath) is composed of a *finite* number N of uncoupled harmonic oscillators (HOs), characterizing a structured bath, for which a non-Markovian behavior is expected. Two distinct physical situations are assumed for the system particle: the HO and the Morse potential. In the limit $N \to \infty$ the bath is assumed to have an ohmic, sub-ohmic or super-ohmic spectral density. In the case of the HO, for very low values of N ($\lesssim 10$) the mean energy and purity oscillate between HO and bath indefinitely in time, while for intermediate and larger values ($N \sim 10 \to 500$) they start to decay with two distinct time regimes: exponential for relatively short times and power-law for larger times. In the case of the Morse potential we only observe an exponential decay for large values of N while for small N's, due to the anharmonicity of the potential, no recurrences of the mean energy and coherences are observed. Wave packet dynamics is used to determine the evolution of the particle inside the system potentials. For both systems the time behavior of a non-Markovianity measure is analyzed as a function of N and is shown to be directly related to the time behavior of the purity.

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1. Introduction

The quantum dynamics of the physically relevant part in a complex system can be described as the dynamics of few degrees of freedom (the main system) coupled to many degrees of freedom which effectively act as a bath or environment, which may induce dissipation and decoherence [1]. In such a description the bath itself can be highly structured, containing specific modes which strongly influences back the system dynamics. Structured baths have become of significance since they describe realistic situations of non-equilibrium physics. Three major recent examples are the single localized spin 1/2 coupled to a finite spin-polarized environment [2], superconducting quantum bit coupled to an environment composed of a single electromagnetic mode of the cavity [3], and the energy transfer between a light-harvesting protein and a reaction center protein [4]. Understanding the physics encountered in this process will help exploring its huge potential [5]. Thus, theoretical descriptions of general features involving decoherence and quantum energy exchanges of the main system coupled to structured baths are of relevance for non-equilibrium physics processes. The present work is an attempt of such description.

The quantum dissipation and decoherence are analyzed for an open system interacting with its environment by collision processes. The problem (System + Environment + Interaction) is conservative but, due to energy exchange between system and environment, the *system* can be seen as an open system with dissipation. Such a theoretical model has been proposed and studied in quantum [6–8] and classical [7–9] systems. Various models were developed to treat such open systems. We start by mentioning the methods which have focused on an explicit quantum dynamical treatment of the system + bath dynamics: path integral approaches [10–12], the multiconfiguration time-dependent Hartree (MCTDH) technique for wave packet propagation [13], the Gaussian-MCTDH approach [1], the effective-mode representation[14], and the local coherent-state approximation to system–bath dynamics [15]. Another way of studying the system + bath dynamics is to solve the non-Markovian master equations [16–18], including some semiclassical approaches [19,20].

Here a non-Markovian quantum trajectory theory is used, named non-Markovian quantum-state diffusion, that describes the dynamics of a quantum system coupled linearly via position to an environment [21–24]. Differently from most of the previous studies, the environment here is composed by a *finite* number N of uncoupled HOs, as studied recently for classical continuous systems [25,26] and maps [27]. In such cases we say to have a discrete or structured bath. As discussed later, such a discrete bath may induce a non-Markovian evolution in the system. Some experiments in which the non-Markovian behavior arises due to the discreteness of the bath can be mentioned: high-Q microwave cavities, quantum optics in materials with a photonic band gap, output coupling from a Bose–Einstein condensate to create an atom laser [28–32] or the decoherence phenomenon [33–36]. From the classical point of view, in the context of finite baths with uncoupled HO, there are some works which analyze the effect of discrete (structured) baths on the system energy decay [9,25,26] and on ratchet transport [37,38]. The main result found is that finite baths may induce a non-Markovian dynamics on the system particle. From the quantum point of view, most works [1,9,15,20,36,39] focus on the analysis of changing the frequency distributions and the coupling strength between system and bath. In a distinct context analytical results [40] studied the time evolution of the concurrence and the purity of two interacting qubits embedded in finite and infinite numbers of environmental spins. However, no recurrences are analyzed. Application to finite quantum thermostats was also discussed [41].

We analyze systematically the effect of increasing the number of oscillators N from the bath on the system energy and purity decay. In most cases we vary $N = 1 \to 500$. As N increases, the quantum simulations need long computational times since they were realized over many realizations of the bath. Usually we use 1000 realizations but, when specified, we needed more. For very low values of N the mean time energy and the purity decrease but comes back to the same initial value. This energy exchange (and the purity behavior) between system and bath continues for larger times. For intermediate and larger values of N ($10 \lesssim N \lesssim 500$) the initial energy inside the system and the purity never return back to the system (for the integrated times) and suffer a transition from exponential decays for shorter times to power-law decays for larger times.

The paper is organized as follows. In Section 2 we introduce the basic concepts of non-Markovian quantum-state diffusion and derive a new simplified stochastic Schrödinger equation valid for *finite* baths. In Section 3 the simplified equation is applied to analyze the N dependence of some useful physical quantities such as the energy decay, the average position, and the purity (decoherence). In this section the harmonic potential is considered. In Section 4 a Morse potential is used for the system particle. In the last section we present a summary and the conclusions.

2. Linear non-Markovian quantum-state diffusion

The non-Markovian quantum-state diffusion (QSD) equation is based on a standard model of open system dynamics: a quantum system interacting with a bosonic environment with the total Hamiltonian

$$H_{tot} = H + \sum_{\lambda} g_{\lambda}(La_{\lambda}^{+} + L^{+}a_{\lambda}) + \hbar \sum_{\lambda} \omega_{\lambda} a_{\lambda}^{+} a_{\lambda}, \tag{1}$$

where H is the Hamiltonian of the system of interest, L is a system operator coupling to environment and a_{λ}^{+}, a_{λ} are the raising and lowering operators, with the property $[a_{\lambda}, a_{\lambda'}^{+}] = \delta_{\lambda\lambda'}$. The linear non-Markovian QSD equation [23,24,42–44] is given by

$$\hbar \left| \frac{\partial}{\partial t} \psi_t \right\rangle = -\mathrm{i}H' \left|\psi_t\right\rangle + Lz_t^{*} \left|\psi_t\right\rangle - L^{+} \int_0^t \mathrm{d}s K(t-s) \frac{\delta \left|\psi_t\right\rangle}{\delta z_s^{*}}, \tag{2}$$