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A Bohmian approach to the non-Markovian non-linear Schrödinger–Langevin equation

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ABSTRACT

In this work, a non-Markovian non-linear Schrödinger–Langevin equation is derived from the system-plus-bath approach. After analyzing in detail previous Markovian cases, Bohmian mechanics is shown to be a powerful tool for obtaining the desired generalized equation.

1. Introduction

The theory of open quantum systems is of fundamental importance to properly describe real systems, which do not exist in complete isolation [1,2]. Among the main approaches usually considered to incorporate environmental effects in the dynamics of the system under study, non-linear Schrödinger equations and system-plus-bath techniques are two of the most representative [1]. The second option is usually preferred due to the following facts: (i) the total system can be taken as closed and, therefore, usual techniques can be employed to study the dynamics of the desired system, (ii) it opens up the full quantum mechanical treatment and reduces in the classical limit to an appropriate description in terms of a Langevin equation, (iii) it is based on microscopic approaches which are currently of fundamental importance because of their experimental control. However, there are connections between these two approaches. Specifically, in the Markovian regime with Ohmic friction, the Schrödinger–Langevin or Kostin [3] equation can be derived within the Caldeira–Leggett approach [4] within a system-bath bilinear coupling (see, for example, Ref. [2]). In spite of its

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drawbacks (for instance, breaking of the superposition principle) [5], it is of interest to have a deeper understanding of the Kostin equation. In fact, the interest on it arises because, regardless of the intrinsic nonlinearity given by the logarithmic term, it preserves the norm of the wavefunction. To give an example of its usefulness from a practical side, we mention that it has been recently considered in the context of dissipative time-dependent density functional theory [6] as a way to construct dissipative functionals. Moreover, a very recent and different example of the applicability of non-linear Schrödinger equations can be found in [7,8], where the authors combine two different non-linearities, one of them being Kostin-like and the other incorporating continuous measurements, which can be understood as an energy dissipation operator in an effective Hamiltonian.

When a non-linear function is assumed for the coupling between the system and the bath, state-dependent dissipation and multiplicative noise appear [9,10]. This behavior can be found, for example, in rotational [11] tunneling systems or in the canonical description of chiral molecules [12], among others. In these cases, and considering again the Markovian regime, it has been recently shown that a generalized Schrödinger–Langevin equation (GSLE) can be derived [13] from a Caldeira–Leggett model with non-linear coupling. Therefore, in view of this generalized Kostin-like equation, the next question that arises naturally is: would it be possible to obtain a non-linear and non-Markovian Kostin-like equation? The answer to this question is not only of academic but also of practical interest since memory effects are present in a variety of physical systems (see, for example, Refs. [14–17]). Moreover, following the argumentations found in [6], this non-Markovian Kostin-like equation would constitute a plausible basis towards the incorporation of memory effects in time-dependent density functional theory, which is a powerful tool to simulate large systems.

The paper is organized as follows. In Section 2, we briefly review how to derive the GSLE from the Caldeira–Leggett model in the Markovian case. In Section 3, the main problem of the obtention of a non-Markovian GSLE when the Schrödinger formulation is employed is shown. In Section 4, the Bohmian formulation is considered in order to solve the previous problem and the desired equation is obtained. Finally, in Section 5, a brief summary of the obtained results is given.

2. Preliminaries

Let us consider the Caldeira–Leggett model [4] for a one dimensional system. The generalization to the three dimensional case will be presented at the end of the article. Basically, this approach models a massive particle in a heat bath, consisting of an infinite set of harmonic oscillators. From these considerations, the following total Hamiltonian arises:

$$H_T = H_s + H_b + H_{sb}. \tag{1}$$

The first term is the Hamiltonian of an isolated particle in presence of a potential,

$$H_s = \frac{p^2}{2m} + V(x). \tag{2}$$

The Hamiltonian of the bath is

$$H_b = \frac{1}{2}\sum_i \left(\frac{p_i^2}{m_i} + m_i\omega_i^2 x_i^2 \right), \tag{3}$$

and the coupling between the system and the bath is written as

$$H_{sb} = \sum_i \left[\frac{d_i^2 f^2(x)}{m_i\omega_i^2} - 2d_i f(x) x_i \right]. \tag{4}$$

Originally, although the system-bath coupling, given by the $x_i f(x)$ term, was assumed to be linear by Caldeira and Leggett [4], the function $f(x)$ will be taken to be a generic function of the position of the system. This general case turns to be useful when state-dependent dissipation is needed to simulate the corresponding dynamics [14–17].