Physica A 393 (2014) 155–172

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Non-Markovian expansion in quantum Brownian motion

Eduardo S. Fraga [a,b], Gastão Krein [c], Letícia F. Palhares [d,e,*]

[a] Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, D-60438 Frankfurt am Main, Germany
[b] Instituto de Física, Universidade Federal do Rio de Janeiro, Caixa Postal 68528, 21941-972 Rio de Janeiro, RJ, Brazil
[c] Instituto de Física Teórica, Universidade Estadual Paulista, Rua Dr. Bento Teobaldo Ferraz 271 - Bloco II, 01140-070 São Paulo, SP, Brazil
[d] Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany
[e] Departamento de Física Teórica, Universidade do Estado do Rio de Janeiro, Rua São Francisco Xavier 524, 20550-900 Rio de Janeiro, RJ, Brazil

HIGHLIGHTS

- Role of the frequency cutoff for the interaction of the system with the heat bath.
- Analytic expansion for exact non-Markovian dissipation kernel and colored noise.
- Systematic inclusion of non-local corrections.
- Comparison to the traditional (Markovian) Langevin approach for an exponential kernel.
- Analysis of non-Markovian Brownian motion.

ARTICLE INFO

Article history:
Received 6 August 2012
Received in revised form 14 August 2013
Available online 19 September 2013

Keywords:
Langevin dynamics
Non-Markovian processes
Brownian motion

ABSTRACT

We consider the non-Markovian Langevin evolution of a dissipative dynamical system in quantum mechanics in the path integral formalism. After discussing the role of the frequency cutoff for the interaction of the system with the heat bath and the kernel and noise correlator that follow from the most common choices, we derive an analytic expansion for the exact non-Markovian dissipation kernel and the corresponding colored noise in the general case that is consistent with the fluctuation–dissipation theorem and incorporates systematically non-local corrections. We illustrate the modifications to results obtained using the traditional (Markovian) Langevin approach in the case of the exponential kernel and analyze the case of the non-Markovian Brownian motion. We present detailed results for the free and the quadratic cases, which can be compared to exact solutions to test the convergence of the method, and discuss potentials of a general nonlinear form.

1. Introduction

The quest for understanding the evolution of quantum systems under the influence of an environment towards equilibrium is ubiquitous in theoretical physics. In particular, the study of quantum-mechanical open systems has produced a long list of different techniques and models [1,2]. As a matter of fact, most realistic physical systems will go through a transient nonequilibrium regime before thermalization is achieved. In the equilibration process, interactions with an infinite set of degrees of freedom, which drain energy from the system, usually play a major role. This process can in many cases be

---

[*] Corresponding author at: Departamento de Física Teórica, Universidade do Estado do Rio de Janeiro, Rua São Francisco Xavier 524, 20550-900 Rio de Janeiro, RJ, Brazil.

E-mail addresses: fraga@if.ufrj.br (E.S. Fraga), gkrein@ift.unesp.br (G. Krein), leticiapalhares@gmail.com, leticia@if.ufrj.br (L.F. Palhares).

0378-4371/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.physa.2013.09.018

described stochastically by the use of a Langevin equation [1], and was successfully applied in a variety of situations. For a comprehensive list of references, see Ref. [2].

The microscopic derivation of a Langevin equation in principle yields a dissipation kernel, which encodes memory effects or retardation due to the finite reaction time of the environment, and colored noise. These two contributions are tied together by the fluctuation–dissipation theorem [1]. In a very peculiar limit, namely that of very long times compared to the reaction time, one can use the Markovian approximation in which the dissipation kernel is reduced to a local term and the noise becomes white. For situations in which such a hierarchy of scales appears naturally, or for the cases where one is not interested in the details of transient regimes, this is a very useful simplifying approximation.

On the other hand, there has been an increasing interest in the nonequilibrium dynamics of phase conversion in a number of systems in which transient non-Markovian effects seem to be of relevance. When a precise determination of different and yet similar time scales in the process of thermalization must be achieved, one is obliged to include all the details in the analysis of the dynamics. In most cases the appropriate framework seems to be that of in-medium nonequilibrium field theory [3], especially in applications to the regimes of nucleation and spinodal decomposition after a first-order transition [4] in a myriad of systems, from the formation of the quark–gluon plasma in high-energy heavy ion collisions [5] to primordial phase transitions in the early universe [6]. In the case of ultra-relativistic heavy ion collisions, we have shown that memory effects are important in the determination of the relevant time scales of the phase conversion process for the chiral transition [7] and for the hadronization (confinement) of the deconfined plasma as it expands and cools down below the critical temperature [8], and can significantly affect the spinodal explosion that presumably occurs [9,10], bringing consequences to the phenomenology [7,8].

Since the structure of memory integrals and colored noise that appears in realistic field-theoretic descriptions of the dynamics of phase transitions is often rather complicated [3,11–16], systematic analytic approximations, as well as efficient numerical methods, are called for. In this paper, we are interested in the development of analytic approximations that can also be useful when coupled with numerical methods. We choose to build our approach in the much simpler case of dissipation in quantum mechanics, where all approximations and important scales are under control, and where one also finds a wide variety of applications [2].

For instance, stochastic versions of the Schrödinger equation, which are useful in describing open quantum dynamics have been generalized to their non-Markovian dissipative forms [17,18]. In the case of a harmonic oscillator, in a model that is similar to a non-Markovian quantum Brownian motion [32], one can find an exact solution for certain particular forms of the noise correlator, as shown recently in Ref. [19] for the case of an exponential correlation function.

To quote a very relevant, concrete example in condensed matter physics, consider the description of localization phenomena in low-dimensional disordered quantum systems. The characterization of conductivity properties in a disordered low-dimensional system appears to be well-described by a generalized Langevin equation (GLE) with a fully non-Markovian kernel [20], associated with the predominance of a single frequency in the heat bath [21]. In this case, one cannot disregard *a priori* non-local effects, since they are the essential feature. In this vein, the analysis we present here provides a first step towards a systematic semi-analytic means of estimating non-local contributions in a general semiclassical description of quantum dissipative systems. Memory kernels also appear in models of financial market data [22]. In particular, long-range memory seems to be present in stochastic processes underlying financial time series which can originate from market activity, i.e. the number of trades per unit time [23]. In chemical and biological problems Langevin equations with a memory kernel are also ubiquitous. For example, the equilibrium fluctuation of the distance between an electron transfer donor and an acceptor pair within a protein molecule [24] has been shown to undergo subdiffusion and has been modeled by a GLE [25]. More recently, the transition from Markovian to non-Markovian regimes in the dynamics of open quantum systems has been studied experimentally in a controlled all-optical setup [26].

The framework that is particularly suited for the integration over degrees of freedom associated with the heat bath, and that is most amenable to generalization to field theory is that of path integrals [27,28]. In particular, it has been very successful in applications to the case of the Brownian motion [2,29–32].

In this paper we study the effects of non-Markovian corrections to the dynamics of a dissipative metastable system in quantum mechanics. Starting from the nonequilibrium evolution of a particle coupled linearly to a set of harmonic oscillators in the Caldeira–Leggett fashion, we study the effects of the non-local dissipation kernel as well as the colored noise that appear in the complete Langevin equation for the particle coordinate in space, $q(t)$. The memory kernel has its origin in the Feynman–Vernon influence functional of the heat bath [33] and is generally too complicated to be treated analytically. In the case of field theory, even a numerical analysis is in most cases quite involved.

To approach the kernel in a simpler, analytic way we develop a systematic expansion in time derivatives of q whose convergence is regulated by increasing powers of the frequency cutoff in the distribution of oscillators, Ω. Physically, above a certain maximum frequency the quantum particle should be "blind" to the bath of oscillators. As we will discuss later, one can implement this cutoff in a variety of equivalent ways, in the sense that the only relevant parameter to control the time correlation is the width of the distribution. Nevertheless, not all cutoff functional forms are allowed if one is concerned with recovering the usual Markovian Langevin dynamics, with a white noise, in the limit $\Omega t \to \infty$. Reasonable choices always yield localized kernels, allowing for truncations in the derivative expansion that are consistent with the fluctuation–dissipation theorem order by order.