Physics Letters A 382 (2018) 1262–1267

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Dynamics of a spin-boson model with structured spectral density

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ARTICLE INFO

Article history:
Received 6 February 2018
Received in revised form 6 March 2018
Accepted 12 March 2018
Available online 15 March 2018
Communicated by M.G.A. Paris

Keywords:
Structured spectral density
Spin-boson model
Bath correlation functions

ABSTRACT

We report the results of a study of the dynamics of a two-state system coupled to an environment with peaked spectral density. An exact analytical expression for the bath correlation function is obtained. Validity range of various approximations to the correlation function for calculating the population difference of the system is discussed as function of tunneling splitting, oscillator frequency, coupling constant, damping rate and the temperature of the bath. An exact expression for the population difference, for a limited range of parameters, is derived.

1. Introduction

The spin-boson model is one of the most prominent models used to study dissipative and decoherence effects in quantum mechanics [1,2]. It describes a two-state system (TSS) coupled to an infinite array of non-interacting harmonic oscillators whose effect on the system is characterized by spectral density $J(\omega)$. The spin-boson model with a power law spectral density, which is the general setting of the model, contains only the cutoff frequency of the bath as an internal energy scale and leads to scale-free-rates while the so-called structured environments provide a more non-trivial internal dynamics which might be relevant for controlling coherence and relaxation times by engineering a properly structured environment [3]. Garg, Onuchic and Ambegaokar (GOA) have shown that the spin-boson model with Ohmic spectral density can be mapped to the problem of a TSS interacting with a harmonic oscillator which is damped by an Ohmic environment whose effective spectral function can be approximated as Lorentzian when the cutoff frequency of the Ohmic bath is much larger than the characteristic frequency of the harmonic oscillator [4]. The GOA model has been used in many studies to describe several phenomena such as electron transfer reactions in various condensed phase environments. The same Hamiltonian and $J(\omega)$, also, describe experimentally relevant quantum systems, such as flux-qubit read out by a dc-SQUID [5–7], atom-based cavity quantum electrodynamics [8], circuit quantum electrodynamics with superconducting systems [9], semiconducting quantum dots in nano-cavities [10] and in nano-mechanical resonators [11,12]. The same model is employed in chemical physics context to study charge transfer [13,14], energy transfer dynamics in photosynthesis [15–17] and linear and nonlinear spectroscopies [14].

Theoretical approaches used to investigate the dynamics of the coupled TSS-damped harmonic oscillator (HO) system can be, broadly, divided into two groups; on the one hand, the infinite dimensional TSS-HO Hamiltonian is approximated by a finite dimensional system which is reduced to Jaynes–Cummings or ac-Stark Hamiltonian depending on whether one is in the resonant or dispersive regime [18]. On the other hand, the problem could be considered as a spin-boson model with a peaked spectral density. A large number of computational techniques have been developed to investigate the dynamics of spin-boson model, such as hierarchical equations of motion, renormalization group techniques and path integral based formalism [13,16,19–22]. The effects of structured spectral density on the decoherence properties of a qubit have been studied with a perturbative approach in Refs. [23,24]. Thorwart et al. have used ab initio QUAPI technique to show that perturbative treatment breaks down when qubit-HO coupling is strong ($g \gg \Gamma$) and when the qubit and the oscillator frequencies are comparable [25]. Gan, Huang and Zheng have studied the dynamics of the spin-boson model by using a unitary transformation method [26] while Ref. [20] has investigated the dephasing times for the TSS-HO system by using flow-equations renormalization method and shown that harmonic oscillator frequency can be used to control qubit dynamics.

As the interaction between the TSS and its environment, whether a bath of non-interacting harmonic oscillator or the damped harmonic oscillator, is considered to be linear, the spectral density function $J(\omega)$ and the bath temperature completely

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https://doi.org/10.1016/j.physleta.2018.03.021

characterizes the TSS-bath coupling. All relevant computational techniques make use of bath correlation function $G(t)$ which is the thermal average of the force auto-correlation of the bath degrees of freedoms or its two-times integrated form to account for the effect of the bath. So, obtaining manageable analytical expressions for $G(t)$ might be beneficial for theoretical as well as computational techniques used to treat the spin-boson problem. There has been a number of reports on the analytical expressions for correlation functions of peaked spectral density [4,27–29]. Nesi, Grifoni and Paladino have studied the dynamics of the system for the large Q-factor oscillator at arbitrary detuning and finite temperatures and obtained analytical expressions for the TSS population [28] for the weak-coupling regime. Building on the findings of Ref. [28], Vierheilig, Bercioux and Grifoni have considered the dynamics of a qubit coupled to a nonlinear oscillator which is coupled to an Ohmic bath and showed that the system can be mapped to the TSS-damped harmonic oscillator model with an effective peaked spectral density [29].

In the present study, our first aim is to obtain an exact analytical expression for the correlation function $G(t)$ of TSS-HO system which is characterized by a peaked spectral density. The TSS-HO system has several characteristic times set by the energy splitting and tunneling amplitude of the TSS, frequency and the damping of the harmonic oscillator, the temperature of the HOs environment and the coupling constant between the HO and the TSS. The complicated interplay among these rate constants make it difficult to develop a universal computational technique which is applicable for all parameter values. Using the derived $G(t)$ expression, we investigate the population dynamics of the TSS and map the validity range of various approximations as function of TSS tunneling splitting, coupling strength between the TSS and the harmonic oscillator, damping of the oscillator and the temperature of the bath. It is found that for a range of parameters, one can use Markov approximation and obtain an exact expression for the population difference.

The outline of the paper is follows: In Section 2, we describe the problem and derive the expression for $G(t)$ and present several approximations to it. The validity range of the approximations is discussed in Section 3 and a brief summary of the study is presented in the conclusions.

2. The model

Let the total Hamiltonian of the closed system be

$$H = \frac{\epsilon_0}{2}\sigma_z + \frac{V}{2}\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \sigma_z \sum_k g_k \left(b_k^\dagger + b_k\right), \tag{1}$$

where ϵ_0 is the splitting of the energy levels of the system, V is the tunneling matrix element and σ_i are the Pauli spin matrices. The bath is modeled as a collection of harmonic oscillators with creation (annihilation) operators $b_k^\dagger$ (b_k) and the mode frequency ω_k. The dynamics of the two-state system are characterized by the population difference $P(t)$ which is defined as the expectation value of σ_z as $P(t) = \mathrm{Tr}_{\mathrm{TSS}}\left[\sigma_z \mathrm{Tr}_{\mathrm{B}}\left(e^{-iHt}\rho(0)e^{iHt}\right)\right]$. Here, $\rho(0)$ is the initial density matrix of the total system which is assumed to be in factorized form $\rho(0) = \rho_{\mathrm{TSS}}(0) \otimes \exp(-\beta H_{\mathrm{B}})/Z$ and the two partial trace operations refer to trace over the bath (B) and system (TSS) degrees of freedom. $P(t)$ for the spin-boson problem obeys the generalized master equation [1]:

$$\frac{dP(t)}{dt} = -\int_0^t dt' \left(K^s(t,t')P(t') + K^a(t,t')\right), \tag{2}$$

where $K^a(t,t')$ and $K^s(t,t')$ are the asymmetric and symmetric parts of the kernel, respectively. They are derived from the two-time integrated bath correlation function $G(t)$

$$G(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \,\langle F(t_2)F(0)\rangle_T + iE_r t, \tag{3}$$

and can be represented as a series in tunneling amplitude V. In Eq. (3), E_r is the reorganization energy of the bath and $\langle F(t)F(0)\rangle_T$ is the thermal average of the force auto-correlation function of the bath modes which is defined as:

$$\langle F(t)F(0)\rangle_T = \frac{1}{2\pi}\int_0^\infty J(\omega)\frac{\cosh(\omega/2k_BT - i\omega t)}{\sinh(\omega/2k_BT)}\,d\omega. \tag{4}$$

The effect of the environment on the system is characterized by bath spectral function $J(\omega)$, which we assume to be of the form

$$J(\omega) = 8\kappa^2 \frac{\gamma\,\omega_0\,\omega}{\left(\omega^2-\omega_0^2\right)^2 + 4\gamma^2\omega^2}, \tag{5}$$

for the present study. $J(\omega)$ in Eq. (5) is a structured spectral function and can be used to describe various types of environments, such as the traditional spin-boson model with an Ohmic environment [4], a TSS coupled to a nonlinear, damped-oscillator [29], or an environment that contains both a background vibrations and one prominent vibrational mode. Depending on the model it describes, its parameters (ω_0, κ, and γ) would have slightly different meanings. Here, we have a two-state system in contact with a harmonic oscillator which damped by an Ohmic thermal bath in mind. So, ω_0 is the frequency of the central harmonic oscillator, κ is the TSS-HO coupling constant, γ is the broadening of the oscillator levels due to its interaction with the Ohmic environment. One should note that $J(\omega)$ of Eq. (5) reduces to so called Debye form in the over-damped limit $\omega_0 \ll \gamma/2$.

The reorganization energy E_r is defined as

$$E_r = \frac{1}{2\pi}\int_0^\infty \frac{J(\omega)}{\omega}\,d\omega, \tag{6}$$

and is equal to κ^2/ω_0 for the spectral density given in Eq. (5). The bath correlation function $G(t)$ can be simplified for the strong coupling regime $\kappa \gg \omega_0$, where one can invoke the short-time approximation by noting that the kernel function $G(t)$ is non-zero only for a very short time and obtain [4]:

$$G_{\mathrm{st}}(t) = \left\langle F(0)^2\right\rangle t^2 + i\,E_r\,t, \tag{7}$$

where $\left\langle F(0)^2\right\rangle$ can be evaluated from Eq. (3) by using Eq. (5) as

$$\left\langle F(0)^2\right\rangle = 2\frac{E_r}{\beta} + \frac{1}{\pi}\frac{E_r\omega_0^2}{\Delta}\,\mathrm{Im}\left[\psi\left(1 + i\tilde{\beta}(\Delta - i\gamma)\right)\right], \tag{8}$$

where $\Delta = \sqrt{\omega_0^2 - \gamma^2}$, $\tilde{\beta} = \beta/(2\pi) = 1/(2\pi k_B T)$ is the inverse temperature scaled by $1/(2\pi)$ and $\psi(z)$ is the complex di-gamma function. To evaluate $G(t)$ for the general case, we write the force auto-correlation function as:

$$\langle F(t)F(0)\rangle_T = \frac{1}{2\pi}\int_0^\infty J(\omega)\left(\coth(\beta\omega/2)\cos(\omega t) - i\sin(\omega t)\right)\,d\omega. \tag{9}$$

One should note that the auto-correlation function is the difference of the Fourier cosine and sine transforms of $J(\omega)\coth(\beta\omega/2)$ and