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Quantum dynamics of a qubit coupled with a structured bath

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Received 8 March 2008, in final form 16 August 2008

Published 4 September 2008

Online at stacks.iop.org/JPhysCM/20/395233

Abstract

The dynamics of an unbiased spin-boson model with Lorentzian spectral density is investigated theoretically in terms of the perturbation theory based on a unitary transformation. The population difference $P(t)$ and susceptibility $\chi''(\omega)$ are calculated for both the off-resonance case $\Delta \lesssim 0.5\Omega$ and the on-resonance case $\Delta \sim \Omega$. The approach is checked by Shiba's relation and the sum rule. As well, the coherent–incoherent transition point α_c can be determined.

1. Introduction

Quantum computation has shown a lot of advantages in performing certain tasks [1, 2]. As the basis of a quantum computer, a quantum bit (qubit) is one of the most attractive research topics today. Qubits were realized many years ago by using microscopic degrees where the decoherence was small enough to exhibit quantum coherence [3, 4]. However, those qubit schemes are difficult to implement for the desired large numbers of interacting qubits which would be of practical value for computation [5]. Therefore, many scalable qubit schemes such as charge, phase and flux qubits are proposed and realized in the last decade [6–8]. Among them, the macroscopic qubit schemes, which were first proposed in Leggett's pioneering work [9], aroused a lot of interest not only for its potential application in quantum computation, but also for its theoretical importance in understanding the boundary between classical and quantum physics.

Since the decoherence is still the biggest problem of quantum computation and quantum information, many of the proposed schemes have a common feature, to minimize the decoherence. That is, the qubit is designed to be not directly coupled to the multi-mode dissipative environment but to a few quantum modes which themselves are coupled to a dissipative environment [8, 10]. In this paper, we focus on the dynamics of a qubit indirectly dissipated by a multi-mode bosonic bath via a quantum oscillator. This model can be interpreted as a flux qubit detected by a SQUID, where the LC resonance circuit acts as a harmonic oscillator (HO) and the current noise is the source of the dissipative environment [8]. It can also describe a qubit placed in a leaky cavity where the single cavity mode act as an HO and the cavity loss is the dissipation [10]. It has been

proved that such a spin-oscillator-bath model can be mapped to a spin-boson model (SBM) with a structured bath such as a bath of Lorentzian form [11–14]:

$$J(\omega) = \frac{2\alpha\omega\Omega^4}{(\Omega^2 - \omega^2)^2 + (2\pi\Gamma\omega\Omega)^2}. \quad (1)$$

The SBM with a conventional bath, such as ohmic bath, piezoelectric bath, etc, can describe a qubit dissipated by a non-interacting multi-mode environment, and it has been studied intensively by various methods [15–17]. However, such a Lorentzian form of bath poses challenge to most of those methods, especially in the large dissipative condition [18]. Until now, the effect of such a structured spectral density has been studied by the quasi-adiabatic propagator path integral (QUAPI) [19], the flow-equation method [18, 20] and the non-interacting blip approximation (NIBA) [18, 21]. The coherence–decoherence transition point has not been provided so far, which means the large dissipative case has not been studied well enough. However, in most scalable qubit schemes realized today, the dissipations are always very large, so a method that can work under severe dissipation would be important in understanding qubit behavior [22]. In the present work, we study this problem in terms of the perturbation treatment based on a unitary transformation. This method, which was proposed by Zheng [23], can lead to analytical results for the population difference and susceptibility. The coherence–decoherence transition point α_c can thus be obtained. Since the unitary transformation reasonably separates the dominant part and the lesser one, even though it is a second-order perturbation method, it still works well for a wide parameter range.

This paper is organized as follows. In section 2, we present the model and introduce our method briefly. In section 3, we calculate the population difference $P(t)$ and compare the results with those of the other methods. In section 4, the susceptibility is calculated and a validation of Shiba's relation is given. In section 5, the coherence–decoherence transition point α_c is studied.

2. Model and treatment

We characterize the qubit by a pseudospin-1/2 operator σ_x as usual (unbiased condition) and the dissipative environment by a multi-mode bosonic bath. Assuming all the couplings to be linear, the qubit-HO–bath interaction Hamiltonian can be written as ($\hbar = 1$)

$$H = -\frac{\Delta}{2}\sigma_x + \frac{P^2}{2M} + \frac{M\Omega^2}{2}(X + q\sigma_z)^2 + \sum_k \left[\frac{\tilde{p}_k^2}{2\tilde{m}_k} + \frac{\tilde{m}_k\tilde{\omega}_k^2}{2} \left(\tilde{x}_k + \frac{\tilde{c}_k X}{\tilde{m}_k\tilde{\omega}_k} \right)^2 \right], \quad (2)$$

where Δ represents the frequency of tunneling between the two states of the qubit, Ω is the frequency of HO, $\tilde{\omega}_k$'s are the frequencies of each mode of the bosonic bath ($k = 1, 2, 3, \dots$) and $q\sigma_z$ is the displacement of the qubit caused by the interaction with the HO, which also has a displacement of $\tilde{c}_k X / (\tilde{m}_k \tilde{\omega}_k)$ caused by the interaction with the bath. According to the procedure of second quantization, the Hamiltonian becomes [20]

$$H = -\frac{\Delta}{2}\sigma_x + \Omega B^\dagger B + \sum_k \tilde{\omega}_k \tilde{b}_k^\dagger \tilde{b}_k + (B^\dagger + B) \times \left[g\sigma_z + \sum_k \kappa_k (\tilde{b}_k^\dagger + \tilde{b}_k) \right] + (B^\dagger + B)^2 \sum_k \frac{\kappa_k^2}{\tilde{\omega}_k}, \quad (3)$$

where B (or B^\dagger) and \tilde{b}_k (or \tilde{b}_k^\dagger) are the annihilation (or creation) operators of the HO and bath, g and κ_k are the coupling constants. The effect of the bath is fully defined by the spectral density, which is assumed to be of ohmic form: $\tilde{J}(\omega) \equiv \sum_k \kappa_k^2 \delta(\omega - \tilde{\omega}_k) = \Gamma \omega \theta(\omega_c - \omega)$.

Such a Hamiltonian can be mapped to the conventional spin-boson model [11, 12]:

$$H = -\frac{\Delta}{2}\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \frac{1}{2}\sigma_z \sum_k g_k (b_k^\dagger + b_k), \quad (4)$$

where the spin dynamics depends only on the Lorentzian structured spectral density $J(\omega)$ given by equation (1) with $\alpha = 8\Gamma g^2 / \Omega^2$. Note that, when the characteristic frequency Ω is higher than the others, say $\Omega > 2\Delta$, $J(\omega)$ is nearly the same as the ohmic spectral density which has been extensively studied. This case will be called off-resonance. For the on-resonance case $\Omega \sim \Delta$, the physical properties of the coupling system with Lorentzian structured spectral density may be quite different from those of the ohmic bath.

According to Zheng's proposal [23], we apply a unitary transformation to the Hamiltonian (4): $H' = \exp(S)H \exp(-S)$, with the generator $S \equiv \sum_k \frac{g_k}{2\omega_k} \xi_k (b_k^\dagger - b_k)\sigma_z$. If $\xi_k = 1$, it reduces to the usual polaron transformation.

After the unitary transformation, the Hamiltonian can be decomposed into three parts:

$$H'_0 = -\frac{\sigma_x}{2}\eta\Delta + \sum_k \omega_k b_k^\dagger b_k - \sum_k \frac{g_k^2}{4\omega_k} \xi_k (2 - \xi_k), \quad (5)$$

$$H'_1 = \frac{\sigma_z}{2} \sum_k g_k (1 - \xi_k) (b_k^\dagger + b_k) - \frac{i\sigma_y}{2} \eta \Delta X, \quad (6)$$

$$H'_2 = -\frac{\sigma_x}{2} \Delta \{ \cosh X - \eta \} - \frac{i\sigma_y}{2} \Delta \{ \sinh X - \eta X \}, \quad (7)$$

where $X \equiv \sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k)$ and η is the thermodynamic average of $\cosh X$. In the limit of zero temperature it is

$$\eta = \exp \left[- \sum_k \frac{g_k^2}{2\omega_k^2} \xi_k^2 \right]. \quad (8)$$

Obviously, H'_0 can be solved exactly since the spin and bosons are decoupled in H'_0 . $\eta\Delta$ gives a rough approximation of the renormalized qubit frequency and $(\eta - 1)\Delta$ is the corresponding Lamb shift of the qubit due to the coupling to the bath. The eigenstate of H'_0 can be expressed as a direct product $|s\rangle| \{n_k\} \rangle$, where $|s\rangle$ is the eigenstate of σ_x and $| \{n_k\} \rangle$ is the eigenstate of the phonons, which means that there are n_k phonons for mode k . Therefore, the ground state of H'_0 is given by $|g_0\rangle = |s_1\rangle| \{0_k\} \rangle$, where $|s_1\rangle$ is the lower eigenstate of the spin and $| \{0_k\} \rangle$ stands for the vacuum state of the bosons.

The choice of η in equation (8) ensures H'_2 contains only the terms of two-boson and multi-boson non-diagonal transitions and its contribution to physical quantities is $(g_k^2)^2$ and higher. Therefore, H'_2 can be omitted in the following discussion. In order to minimize H'_1 , we let $H'_1|g_0\rangle = 0$, and the parameters ξ_k 's are determined as

$$\xi_k = \frac{\omega_k}{\omega_k + \eta\Delta}. \quad (9)$$

Note that $0 \leq \xi_k \leq 1$ measures the intensity of the spin-boson coupling $\xi_k \sim 1$ if the boson frequency ω_k is larger than the renormalized tunneling $\eta\Delta$, but $\xi_k \ll 1$ for $\omega_k \ll \eta\Delta$. Since the transformation generated by S is a displacement, physically, one can see that high-frequency bosons ($\omega_k > \eta\Delta$) follow the tunneling particle adiabatically because the displacement is $g_k \xi_k / \omega_k \sim g_k / \omega_k$. However, bosons of low-frequency modes $\omega_k < \eta\Delta$ in general are not always in equilibrium with the tunneling particle, hence the particle moves in a retarded potential arising from the low-frequency modes. When the non-adiabatic effect dominates, $\omega_k \ll \eta\Delta$, the displacement $\xi_k \ll 1$. In addition, because of such a choice of ξ_k , H'_1 is automatically of rotating-wave form:

$$H'_1 = \sum_k V_k (b_k^\dagger \sigma_- + b_k \sigma_+), \quad (10)$$

where $V_k = \eta\Delta g_k \xi_k / \omega_k = g_k \eta\Delta / (\omega_k + \eta\Delta)$ and $\sigma_\pm \equiv (\sigma_x \mp i\sigma_y) / 2$. Actually, some effect of the anti-rotating-wave terms has been taken into account in H'_1 by the unitary transformation which is embodied in the renormalized coupling constant V_k .

3. The population difference

The population difference $P(t)$ is defined as $P(t) = \langle \phi(t) | \sigma_z | \phi(t) \rangle$ and $|\phi(t)\rangle$ is the wavefunction in the Schrödinger picture. We choose the initial state as $|+\rangle|b, +\rangle$, where $|+\rangle$ is the eigenstate of $\sigma_z = +1$ and $|b, +\rangle$ is the state of bosons adjusted to the state of $\sigma_z = +1$. Because of the unitary transformation, the population difference $P(t)$ can be written as

$$P(t) = \langle \{0\} | \langle + | e^{iH't} \sigma_z e^{-iH't} | + \rangle | \{0\} \rangle. \quad (11)$$

In the zero-temperature limit, second-order perturbation can be applied to the transformed Hamiltonian and the population difference is given by [23]

$$P(t) = \text{Re} \left\{ \frac{1}{4\pi i} \oint \frac{dE' e^{-iE't}}{E' - \eta\Delta - R(E') + i\gamma(E')} \right\}. \quad (12)$$

The contour of the integrand in equation (12) is composed of a straight line located on the real axis and a semicircle below the real axis with infinite radius. The direction of the contour is anti-clockwise. $R(E')$ and $-\gamma(E')$ in equation (12) are the real and imaginary parts of $\sum_k V_k^2 / (E' + i0^+ - \omega_k)$ and they can be written as

$$R(\omega) = \int_0^\infty d\omega' \frac{(\eta\Delta)^2 J(\omega')}{(\omega' + \eta\Delta)^2 (\omega - \omega')}, \quad (13)$$

$$\gamma(\omega) = \pi(\eta\Delta)^2 J(\omega) / (\omega + \eta\Delta)^2. \quad (14)$$

We should emphasize that the integral expression in equation (12) is an exact one under our second-order approximation scheme and it can be done by using the residue theorem approximately. Suppose the poles of the integrand are $E_p = \omega_p - i\gamma_p$: then the population difference becomes

$$P(t) = \sum_p a_p e^{-\gamma_p t} \cos(\omega_p t), \quad (15)$$

where the renormalized qubit frequency ω_p is the solution of the equation

$$\omega - \eta\Delta - R(\omega) = 0, \quad (16)$$

decay rate is $\gamma_p = a_p \gamma(\omega_p)$ and a_p can be interpreted as the weight of each oscillating mode. If there is only one solution of equation (16), then $a_p = 1$. However, if two solutions $\omega_p = \omega_\pm$ appear, then $a_+ = \frac{\eta\Delta - \omega_-}{\omega_+ - \omega_-}$ and $a_- = \frac{\omega_+ - \eta\Delta}{\omega_+ - \omega_-}$.

To check the result, a comparison between our result and the ones of exactly solvable models would make sense. In the limit of small HO–bath coupling ($\Gamma \rightarrow 0$), corresponding to large quality factors of the HO, the spectral density $J(\omega)$ goes to $\frac{8g^2}{\Omega} \delta(\frac{\omega}{\Omega} - \frac{\omega'}{\Omega})$, where $\alpha = 8\Gamma g^2 / \Omega^2$ has been applied. Therefore, from equation (13), $R(\omega)$ goes to $\frac{4g^2(\eta\Delta)^2}{(\Omega + \eta\Delta)^2(\omega - \Omega)}$. According to equation (16), the renormalized qubit frequency ω_p is

$$\omega_p = \frac{\Omega + \eta\Delta}{2} \pm \sqrt{\left(\frac{\Omega - \eta\Delta}{2}\right)^2 + \frac{4g^2(\eta\Delta)^2}{(\Omega + \eta\Delta)^2}} \equiv \omega_\pm. \quad (17)$$

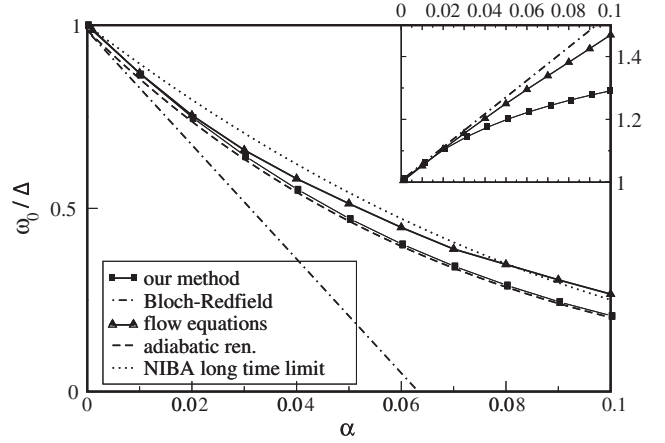


Figure 1. The renormalized tunneling frequency ω_p versus the coupling strength α . Main plot: $\Delta/\Omega = 0.1$, $\Gamma = 0.02$; inset: $\Delta/\Omega = 1.1$, $\Gamma = 0.06$. The results of the other methods are from Wilhelm’s article [18].

Suppose the resonance condition is $\Omega = \eta\Delta$ rather than $\Omega = \Delta$, though the two frequencies $\eta\Delta$ and Δ are nearly the same when Γ is very small. For the resonance condition, where the rotating-wave approximation (RWA) is believed to be valid, we obtain $\omega_\pm = \Omega \pm g$, which fully agrees with the result of the simple Jaynes–Cummings model [24].

In the case of finite detuning $\delta \equiv |\Omega - \eta\Delta|$, and weak coupling between qubit and HO, from equation (17) we find (assuming, e.g., $\Omega > \Delta$)

$$\omega_+ = \Omega + \frac{4g^2\eta^2\Delta^2}{\delta(\Omega + \eta\Delta)^2} \quad (18)$$

$$\omega_- = \eta\Delta - \frac{4g^2\eta^2\Delta^2}{\delta(\Omega + \eta\Delta)^2} \quad (19)$$

yielding $\omega_+ - \omega_- = \delta(1 + \frac{8g^2\eta^2\Delta^2}{\delta^2(\Omega + \eta\Delta)^2})$. Similar as in [21], ω_- can be interpreted as the Stark-shifted qubit frequency due to the coupling with the harmonic mode.

In what follows, we show the renormalized tunneling frequency ω_p calculated numerically from equation (16) for both off- and on-resonance cases without the limitation of weak HO–bath coupling. Here, we only choose the one corresponding to the intrinsic qubit frequency Δ in order to compare with the results of other methods. The main plot in figure 1 describes the off-resonance case. We can see that the tunneling frequency ω_p decreases as the coupling strength α increases. This is similar to the ohmic case because the Lorentzian structured spectral density becomes the ordinary ohmic one for $\Delta/\Omega \ll 1$. However, it is quite different for the on-resonant case with $\Delta \sim \Omega$ (the inset of figure 1). We can see that, as the coupling strength α increases, the tunneling frequency ω_p increases too. It is said that the coupling enhances the tunneling frequency [18].

Note that, in the main plot of figure 1, our calculation of the renormalized qubit frequency ω_0 is very close to the one given by adiabatic renormalization. It may be the result of the similar spirit between the adiabatic renormalization and our method. Both of them consider the high-frequency phonons

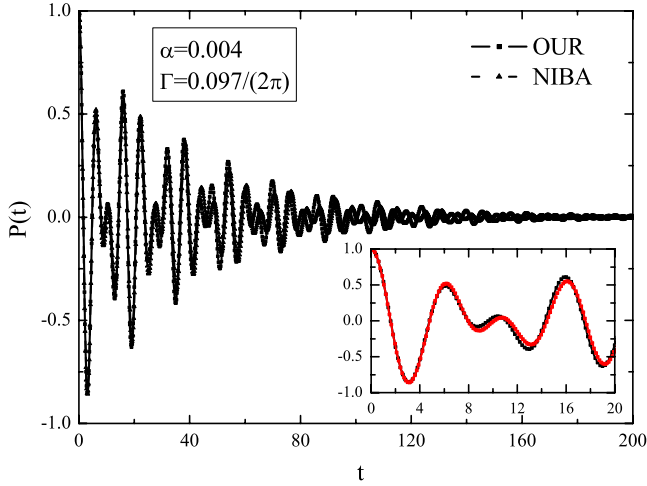


Figure 2. The dynamics of population difference $P(t)$. The parameters are: $\alpha = 0.004$, $\Delta = \Omega$, $\Gamma = 0.097/(2\pi)$. The result of the non-interacting blip approximation (NIBA) method are from Nesi's article [21].

(This figure is in colour only in the electronic version)

can follow the electron adiabatically (see our discussion of ξ_k in section 2). Following the adiabatic renormalization method [25], the renormalized qubit frequency is

$$\tilde{\Delta} = \Delta \exp \left[- \int_{p\tilde{\Delta}}^{\infty} d\omega \frac{J(\omega)}{2\omega^2} \right], \quad (20)$$

where p is some number larger compared to unity. This expression is quite similar to our calculation of $\eta\Delta$:

$$\begin{aligned} \tilde{\Delta} &= \eta\Delta = \Delta \exp \left[- \int_0^{\infty} d\omega \frac{J(\omega)}{2(\omega + \tilde{\Delta})^2} \right] \\ &= \Delta \exp \left[- \int_{\tilde{\Delta}}^{\infty} d\omega \frac{J(\omega - \tilde{\Delta})}{2\omega^2} \right]. \end{aligned} \quad (21)$$

However, we should emphasize that our calculation of ω_0 not only takes the adiabatic phonons into account, but also includes the first-order term H'_1 (see equation (10)), which enables us to calculate the dissipative dynamics of physical quantities. Moreover, from equation (20) we can see that the adiabatic renormalization can never predict the positive change of the tunneling frequency since $\tilde{\Delta}$ is always less than Δ .

In figure 2, the population difference $P(t)$ is calculated according to equation (15) and compared with the result of the non-interacting blip approximation (NIBA) method. Here, the coupling constant α is very small, where the NIBA method is believed to be correct. Our result shows good agreement with NIBA. Note that it is in the on-resonance case and one can see that $P(t)$ shows a double-frequency oscillation. In the following discussion we will see that our method can actually work well for much stronger coupling constant α , no matter if it is in the off-or on-resonance case.

In figure 3, we fix the coupling constant $\alpha = 0.01$ and $\Gamma = 0.02$. The behaviors of $P(t)$ are shown for different ratios Δ/Ω . The curves show that it is only a single-frequency oscillation for the off-resonance case ($\Delta/\Omega \lesssim 0.5$). However, in the on-resonance region ($\Delta \sim \Omega$), $P(t)$ exhibits two characteristic frequencies which are both important to the time evolution of the population difference. In figure 4, we fix it in the case of $\Delta = \Omega$ and $\Gamma = 0.02$. By altering the coupling constant α , the population difference $P(t)$ changes significantly. These curves show that $P(t)$ damps out quickly, just like an over-damping curve as α becomes large enough.

Here, to make it more clear, we summarize the merit of our method compared to NIBA, QUAPI and adiabatic renormalization. Firstly, our method can work under severe dissipation compared to NIBA. Secondly, positive change of the tunneling frequency can be predicted under our framework when $\Delta \approx \Omega$, which can never be predicted by adiabatic renormalization. Finally, our method is mainly analytical,

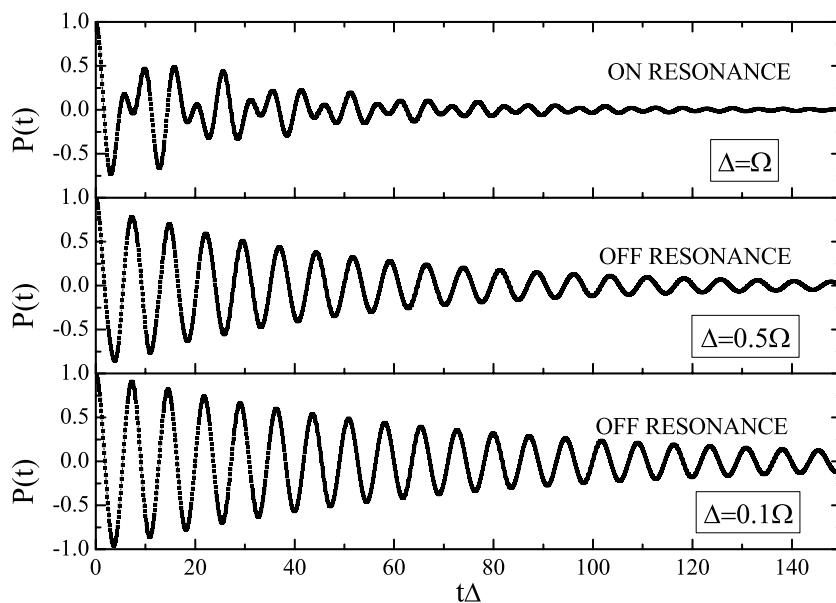


Figure 3. The dynamics of population difference $P(t)$ for different detuning. The parameters are: $\alpha = 0.01$, $\Gamma = 0.02$.

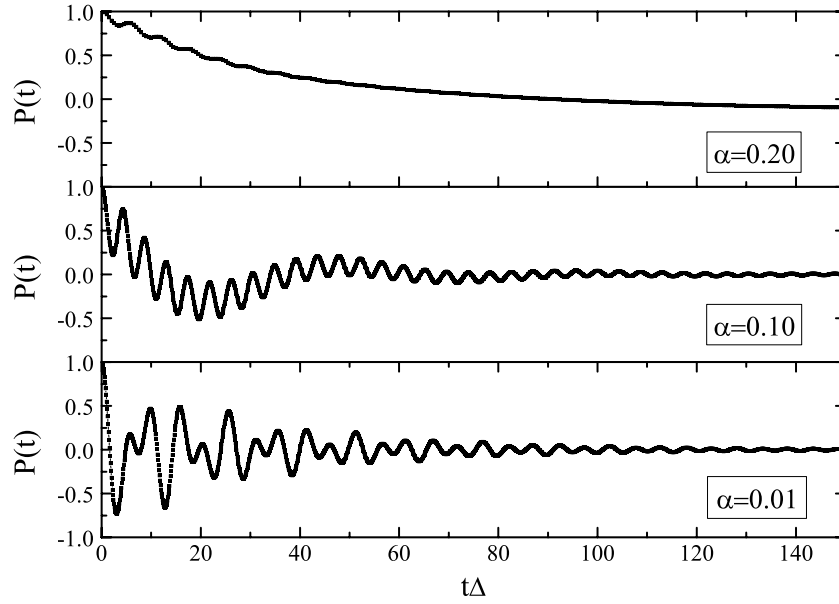


Figure 4. The dynamics of population difference $P(t)$ for different coupling strength α in the on-resonance case. The parameters are: $\Delta = \Omega$, $\Gamma = 0.02$.

which may give more intuitive inspections into this problem compared to QUAPI [19, 26].

4. The susceptibility and Shiba's relation

The retarded Green's function is defined as

$$G(t) = -i\theta(t)\langle[\sigma_z(t), \sigma_z]\rangle_\beta, \quad (22)$$

where $\langle \dots \rangle_\beta$ represents the average with thermodynamic probability $\exp(-\beta H')$ and $[A, B]$ is the commutator $AB - BA$. The Fourier transformation of $G(t)$ is denoted as $G(\omega)$ which satisfies an infinite chain of equations of motion. We make the cutoff approximation for the equation chain at the second order of g_k and the solution for $T = 0$ is [23]

$$G(\omega) = \frac{1}{\omega - \eta\Delta - \sum_k V_k^2/(\omega - \omega_k)} - \frac{1}{\omega + \eta\Delta - \sum_k V_k^2/(\omega + \omega_k)}. \quad (23)$$

The susceptibility $\chi(\omega) = -G(\omega)$, and its imaginary part is

$$\chi''(\omega) = \frac{\gamma(\omega)\theta(\omega)}{[\omega - \eta\Delta - R(\omega)]^2 + \gamma^2(\omega)} - \frac{\gamma(-\omega)\theta(-\omega)}{[\omega + \eta\Delta + R(-\omega)]^2 + \gamma^2(-\omega)}. \quad (24)$$

Define the function $S(\omega)$ as $S(\omega) = \chi''(\omega)/\omega$ with its limit at $\omega \rightarrow 0$ being

$$\lim_{\omega \rightarrow 0} S(\omega) = \frac{2\pi\alpha}{[\eta\Delta + R(0)]^2}. \quad (25)$$

Also, the static susceptibility can be obtained from the imaginary part according to the Kramers-Kronig relation:

$$\chi'(\omega = 0) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\chi''(\omega)}{\omega} d\omega. \quad (26)$$

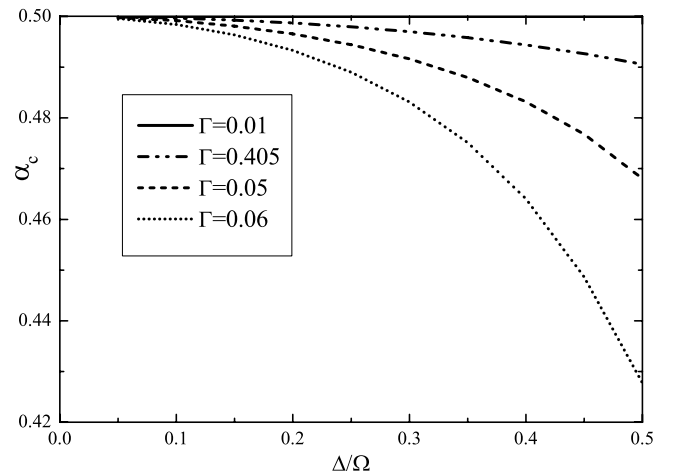


Figure 5. The coherent-incoherent transition point α_c versus Δ/Ω for different Γ .

One can check that Shiba's relation [27–30]:

$$\lim_{\omega \rightarrow 0} S(\omega) = \frac{\pi}{2} \alpha [\chi'(\omega = 0)]^2 \quad (27)$$

is exactly satisfied within the computational precision as long as α is smaller than α_c (see section 5), where a coherent-incoherent transition is believed to occur. Table 1 is the validation of Shiba's relation for some representative parameters.

5. The coherent-incoherent transition

In this section, we confine our discussion to the off-resonant regime ($\Delta \lesssim 0.5 \Omega$). In section 3 we have demonstrated that the tunneling frequency ω_p decreases as the coupling

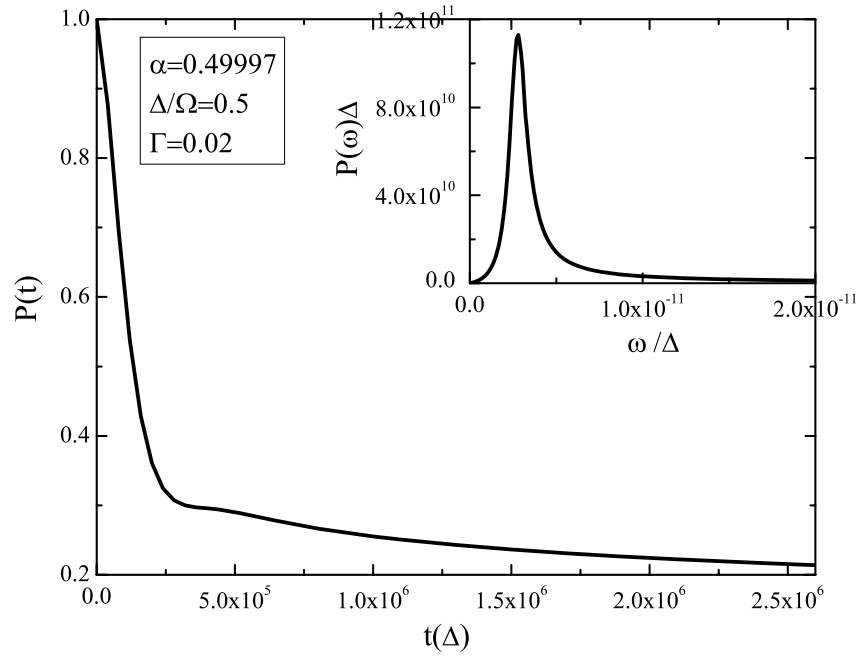


Figure 6. The dynamics of population difference $P(t)$. Main plot: $P(t)$ is very like a over-damping curve. Inset: frequency dependence of population difference. The parameters are: $\alpha = 0.49997$, $\Delta/\Omega = 0.5$, $\Gamma = 0.02$.

Table 1. Shiba's relation are checked for both off- and on-resonance cases.

α	Δ/Ω	Γ	$\lim_{\omega \rightarrow 0} S(\omega)$	$\chi'(\omega = 0)$	$\frac{2}{\pi\alpha} \frac{\lim_{\omega \rightarrow 0} S(\omega)}{[\chi'(\omega=0)]^2}$
0.05	0.5	0.02	1.309 888 805	4.083 873 432	1.000 000 004
0.2	0.5	0.02	1406.318 989	66.906 295 42	1.000 000 002
0.3	0.5	0.02	265 071.3813	749.999 2950	0.999 999 998
0.4	0.5	0.02	341 991 358.2	23 330.155 36	1.000 000 005
0.45	0.5	0.02	$5.168 917 \times 10^{10}$	270 416.7374	1.000 000 022
0.49997	0.5	0.02	$1.728 027 \times 10^{21}$	$4.691 108 \times 10^{10}$	0.999 852 380
0.02	1.1	0.02	0.189 822 271	2.458 103 206	0.999 993 244
0.03	1.1	0.02	0.359 108 802	2.760 528 394	1.000 001 105
0.06	1.1	0.02	1.663 093 714	4.200 714 470	0.999 998 317
0.1	1.1	0.02	15.344 894 38	9.883 756 902	0.999 999 810
0.15	1.1	0.02	15 978.213 81	260.410 5454	0.999 999 903

strength α increases. As α becomes larger and larger, and finally reaches a particular value α_c where ω_p becomes 0, $P(t)$ then is just a pure damping curve according to equation (15). Therefore, at this particular point α_c , a coherent–incoherent transition occurs. By substituting $\omega_p = 0$ into equation (16), α_c can be determined as shown in figure 5. Therefore, α_c represents the transition from a damped oscillation to over-damping. On the other hand, the function $S(\omega)$ obtained in section 4 also shows very specific behavior at the coherent–incoherent transition point. For coherent oscillation, $S(\omega)$ has a double-peak structure symmetrical with respect to $\omega = 0$. However, as soon as the system becomes incoherent, $S(\omega)$ would have only a quasi-elastic peak at around $\omega = 0$. Therefore, the behavior of $S(\omega)$ can also be a check of the coherent–incoherent transition point α_c .

Since this is a perturbation treatment, we must check carefully whether our method is still applicable as α becomes larger and larger. Here, we choose the parameters $\Delta/\Omega = 0.5$ and $\Gamma = 0.02$ to show our checking process. From

equation (16), we have $\alpha_c = 0.49997$. The population difference is depicted at this critical point as shown in figure 6. We find $P(t)$ is almost a over-damping curve at the transition point $\alpha = \alpha_c$ and its Fourier transformation shows that the renormalized tunneling frequency is very close to zero ($< 10^{-11} \Delta$). On the other hand, from figure 7 we can find $S(\omega)$ also confirms this result. At this critical point, $S(\omega)$ transforms from a double-peak structure to a quasi-elastic peak at $\omega = 0$. In addition, by calculating the integral in equation (12) numerically, the sum rule $P(0) = 1$ is always exactly satisfied within the computational precision when α is smaller than α_c . The same thing happens for Shiba's relation (see table 1). Moreover, according to figure 5, we should note that α_c is 1/2 at the scaling limit $\Delta/\Omega \ll 1$, which is the same as predicted by previous authors in the case of an ohmic bath. However, our result demonstrates that, as the system deviates from the scaling limit, the coherent–incoherent transition point α_c is always less than 1/2, which is different from the ohmic case where α_c is always larger than 1/2 for finite Δ [23].

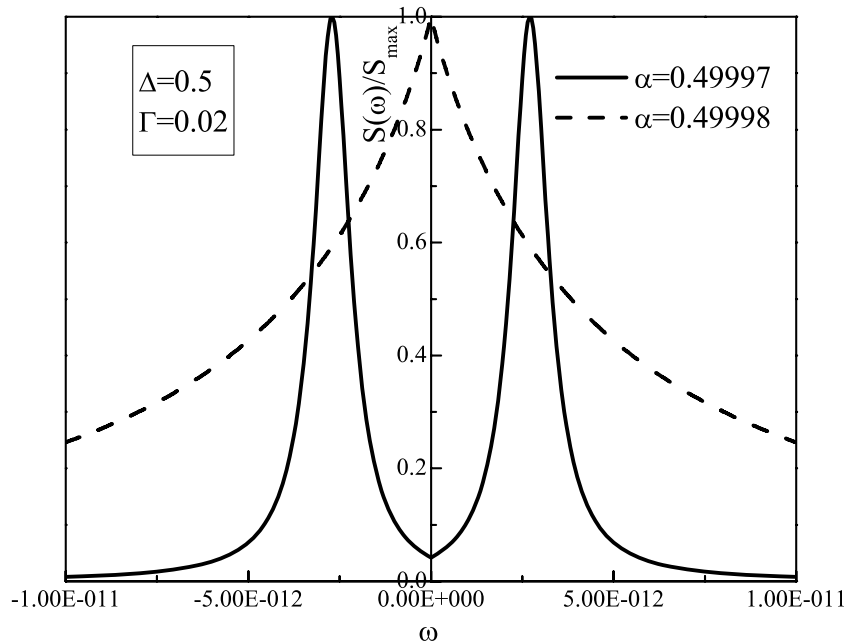


Figure 7. $S(\omega)$ versus ω for different cases. The transition from a double-peak structure of $S(\omega)$ to a quasi-elastic peak indicates the coherent–decoherent transition.

6. Conclusion

The dynamics of an unbiased spin-boson model with Lorentzian spectral density is investigated through a perturbation method based on a unitary transformation. An alternative view of the model is a two-state system coupled to a single harmonic oscillator with frequency Ω , the latter being weakly coupled to an ohmic bath. By comparing with the other approaches, ours shows some advantages: it works well for both the off-resonance case $\Delta \lesssim 0.5\Omega$ and the on-resonance case $\Delta \sim \Omega$, and the coupling constant α may be as large as the coherence–incoherence transition point α_c . We calculate the population difference $P(t)$ and the susceptibility $\chi''(\omega)$, and find the result agrees well with the simple Jaynes–Cummings model for the resonance case $\Omega = \eta\Delta$, under the weak oscillator–bath coupling approximation. The coherent–incoherent transition point α_c is determined, which has not been demonstrated for the structured bath by previous authors to our knowledge. The sum rule and Shiba’s relation are checked carefully as α approaches α_c and they are always exactly satisfied as long as α is smaller than α_c . Admittedly, this method is not suitable for very large system–bath coupling, e.g. $\alpha > \alpha_c$, where the sum rule and Shiba’s relation are no longer satisfied. However, in practical systems a method that works under α_c is good enough since we are always interested in the regime of coherent oscillation.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (grant nos. 10474062 and 90503007).

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