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Analytical approach to the current correlation function in dissipative two-state systems

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Abstract Using the spin-boson model with coupling to Ohmic bath, an analytical approach is developed to study the dynamics of the current correlation function in dissipative two-state systems with the view of understanding the effects of environment and tunneling on the coherent oscillation and the long-time decay of the current correlation function in these systems. An analytic expression of current correlation function is obtained and the results agree very well with that of numerical simulations.

Keywords dissipative two-state systems, coherent-incoherent transition, current correlation function

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1 Introduction

Recently the upsurge of interest in tunneling systems coupled to a dissipative environment has stimulated extensive studies on the physical properties of dissipative two-state systems [1–5]. The dissipative two-state system is important for understanding numerous physical and chemical processes since it provides a universal model for these processes and has been used to describe a large class of problems ranging from Kondo impurities, superconductors, chemical reactions, to amorphous materials [6, 7]. The main interest of these studies has been in understanding how the environment influences the dynamics of the system and in particular how the dissipation de-

stroys quantum coherence [8]. The very recent exploitations of the properties of macroscopic quantum coherence in superconducting quantum interference devices, molecular magnets [9], entanglement of qubit with environment [10] and qubits in quantum computers [11] lead to further interest of theoretical studies on intrinsic physics of this system. While considerable effort has been made to investigate the dynamic equilibrium and non-equilibrium correlations and the Shiba's relation, it is theoretically and experimentally significant to develop an accepted theory for the current correlation function which contains useful informations about excitation spectrum and therefore has been utilized to investigate the absorption spectra and photoluminescence in quantum dot [12] and the spin current in spin-cell device for spintronic circuits [13]. The effect of the environment on small quantum systems can induce mediate coupling of different electronic energy levels and results in many interesting phenomena. However, with the coupling to environment the dissipative two-state system is difficult to handle analytically, which has brought much uncertainty in the interpretation of experimental data and has limited our understanding of many interesting quantum phenomena of two-state systems. Though the dissipative two-state system has been dealt with by using various analytical and numerical methods [6, 7, 14–26], with respect to the current correlation function only numerical calculation has been performed [22]. An analytical study will make it possible to have an insight into the intrinsic properties of dissipative two-state systems. In this work, we focus on the current correlation function of dissipative two-state system by developing an analytical approach to obtain the analytic expression of current correlation function with the view of understanding the effects of environment and tunneling on the dynamic behavior of the current correlation function. The validity of our theory is manifested by the very well agreement of our results with

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that of numerical calculations [22] and, more importantly, this mathematically simple and physically clear method may provide a new analytic method to investigate the absorption spectra and photoluminescence in quantum dots and other confined quantum systems.

2 Analytical approach

The dissipative two-state systems representing tunneling phenomena in a condensed phase are often described by the spin-boson model (SBM) [6, 7]:

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

where Δ is the bare tunneling matrix element and σ_i ($i = x, y, z$) the usual Pauli spin matrices. g_k is the coupling strength of the two-state system to the bath which is represented by an infinite set of harmonic oscillators created by boson operators b_k and b_k^\dagger . The effects of the Ohmic bath and the coupling are completely characterized by the spectral density [7],

$$J(\omega) = \sum_k g_k^2 \delta(\omega - \omega_k) = 2\alpha\omega\theta(\omega_c - \omega) \quad (2)$$

where $\theta(x)$ is the usual step function. The assumption of the Ohmic bath reduces the characteristics of the bath and the coupling to two parameters, the dimensionless coupling (damping) constant α and the upper cutoff ω_c . Though the Hamiltonian (1) seems quite simple, except for some special parameter values, it cannot be solved exactly [26] and up to now there is no single analytical or numerical approach which can produce correct physics for the whole parameter range $0 < \alpha < 1$ and $0 < \Delta < \omega_c$.

The coupling of the system to the dissipative environment leads the tunneling between the two states to lose its phase coherence. The transition from coherent to incoherent dynamics occurs at a critical damping α_c at which the Q factor of the tunneling oscillations vanishes. To take into account the coupling an unitary transformation is applied to H [27–29], $H' = \exp(S)H \exp(-S)$, with the generator

$$S = \sum_k \frac{g_k}{2\omega_k} \xi_k (b_k^\dagger - b_k) \sigma_z \quad (3)$$

The transformation can be done to the end and the result is

$$H' = H'_0 + H'_1 + H'_2 \quad (4)$$

where

$$H'_0 = -\frac{1}{2}\eta\Delta\sigma_x + \sum_k \omega_k b_k^\dagger b_k - \sum_k \frac{g_k^2}{4\omega_k} \xi_k (2 - \xi_k) \quad (5)$$

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

$$H'_2 = -\frac{1}{2} \Delta \sigma_x \left\{ \cosh \left[\sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k) \right] - \eta \right\} - \frac{1}{2} \Delta i \sigma_y \left\{ \sinh \left[\sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k) \right] - \eta \sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k) \right\} \quad (7)$$

The introduced parameters ξ_k and η are determined as follows.

For implementing perturbation treatment conveniently, the transformed Hamiltonian is separated into three parts according to their orders of the coupling strength. The first part H'_0 contains the zeroth-order terms of the transformed Hamiltonian, H'_1 the first-order terms and H'_2 the second as well as higher order terms. Compared with Hamiltonian (1), the tunneling matrix element in the transformed Hamiltonian is renormalized by a factor η , therefore the renormalized tunnelling frequency is given by [26]

$$\Delta_r = \eta \Delta \quad (8)$$

and

$$\eta = \exp \left(- \sum_k \frac{g_k^2}{2\omega_k^2} \xi_k^2 \right) = \exp \left(\frac{\alpha\omega_c}{\omega_c + \eta\Delta} - \alpha \ln \frac{\omega_c + \eta\Delta}{\eta\Delta} \right) \quad (9)$$

η can also be determined by letting $\langle g_0 | H'_2 | g_0 \rangle = 0$, which gives the same result as Eq. (9).

Because of the decoupled form of spin and boson operators, H'_0 can be diagonalized exactly and its eigenstate is a direct product, $|s\rangle | \{n_k\} \rangle$, where $|s\rangle$ is $|s_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ or $|s_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$, i.e., the eigenstates of σ_x , and $| \{n_k\} \rangle$ means that there are n_k phonons for mode k . The ground state of H'_0 is $|g_0\rangle = |s_1\rangle | \{0_k\} \rangle$, where $| \{0_k\} \rangle$ is the vacuum state of bosons in which $n_k = 0$ for every k . H'_1 and H'_2 are treated as perturbation and they should be as small as possible. By letting $H'_1 |g_0\rangle = 0$, the form of ξ_k is determined as

$$\xi_k = \frac{\omega_k}{\omega_k + \eta\Delta} \quad (10)$$

This choice of ξ_k leads to

$$H'_1 = \frac{1}{2}\eta\Delta \sum_k \frac{g_k}{\omega_k} \xi_k \left[b_k^\dagger(\sigma_z - i\sigma_y) + b_k(\sigma_z + i\sigma_y) \right] \quad (11)$$

and the matrix element of H'_1 between $|g_0\rangle$ and other eigenstates of H'_0 to be vanished. Thus H'_1 is related only to the higher-lying excited states of H'_0 and should be irrelevant under renormalization. The total number of phonons of the Ohmic heat bath is usually temperature dependent. At low temperature the multiphonon process is weak and the lowest excited states are $|s_2\rangle|0_k\rangle$ and $|s_1\rangle|1_k\rangle$, where $|1_k\rangle$ is one phonon state with $n_k = 1$ but $n_{k'} = 0$ for all $k' \neq k$. It's easily to check that

$$\begin{aligned} \langle\{0_k\}|\langle s_2|H'_2|g_0\rangle &= 0 \\ \langle 1_k|\langle s_1|H'_2|g_0\rangle &= 0 \\ \langle\{0_k\}|\langle s_2|H'_2|s_1\rangle|1_k\rangle &= 0 \end{aligned} \quad (12)$$

and since $H'_1|g_0\rangle = 0$, we can diagonalize the lowest excited states of H' and rewrite it by means of projective description in Dirac notation as

$$\begin{aligned} H' &= -\frac{1}{2}\eta\Delta|g_0\rangle\langle g_0| + \sum_E E|E\rangle\langle E| \\ &+ \text{terms of higher excited states} \end{aligned} \quad (13)$$

The diagonalization of H' is through the following transformation [16]:

$$|s_2\rangle|\{0_k\}\rangle = \sum_E x(E)|E\rangle \quad (14)$$

$$|s_1\rangle|1_k\rangle = \sum_E y_k(E)|E\rangle \quad (15)$$

The inverse of the transformation formulas Eqs. (14) and (15) is

$$|E\rangle = x(E)|s_2\rangle|\{0_k\}\rangle + \sum_k y_k(E)|s_1\rangle|1_k\rangle \quad (16)$$

Here, the coefficients $x(E)$ and $y_k(E)$ are given by

$$x(E) = \left[1 + \sum_k \frac{V_k^2}{(E + \eta\Delta/2 - \omega_k)^2} \right]^{-1/2} \quad (17)$$

$$y_k(E) = \frac{V_k}{E + \eta\Delta/2 - \omega_k} x(E) \quad (18)$$

with $V_k = \eta\Delta g_k \xi_k / \omega_k$. E 's are the diagonalized excitation energies of H' and they are the solutions of the equation:

$$E - \frac{\eta\Delta}{2} - \sum_k \frac{V_k^2}{E + \frac{1}{2}\eta\Delta - \omega_k} = 0 \quad (19)$$

derived from the normalization condition $\langle E|E\rangle = 1$. The real and imaginary parts of the third term in left side of Eq. (19) can be calculated by the residue theorem as

$$\sum_k \frac{V_k^2}{E + \frac{1}{2}\eta\Delta - \omega_k \pm i0^+} = R(\Omega) \mp i\gamma(\Omega) \quad (20)$$

where

$$\begin{aligned} R(\Omega) &= P \sum_k \frac{V_k^2}{\Omega - \omega_k} \\ &= -\frac{2\alpha(\eta\Delta)^2}{(\Omega + \eta\Delta)^2} \left\{ \frac{\omega_c(\Omega + \eta\Delta)}{\omega_c + \eta\Delta} \right. \\ &\quad \left. - \Omega \ln \left[\frac{\Omega(\omega_c + \eta\Delta)}{\eta\Delta(\omega_c - \Omega)} \right] \right\} \end{aligned} \quad (21)$$

$$\begin{aligned} \gamma(\Omega) &= \pi \sum_k V_k^2 \delta(\Omega - \omega_k) \\ &= 2\alpha\pi \frac{\Omega(\eta\Delta)^2}{(\Omega + \eta\Delta)^2} \end{aligned} \quad (22)$$

Here P denotes a Cauchy principal value and a change of the variable $\Omega = E + \eta\Delta/2$ is made in evaluations.

The variational ground state energy is supposed to be $E_g = \langle s_1|\langle\{0_k\}|H'|s_1\rangle|\{0_k\}\rangle$. ξ_k can also be obtained by variational principle to minimize E_g and the result obtained in this way is same as Eq. (10).

3 The current correlation function

Our theory, though simple, has been successful in obtaining exact results of the coherence-incoherence transition point $\alpha_c=1/2$ at the scaling limit and the delocalized-localized transition point $\alpha_l = 1$ in Ohmic case which are the well established values and well known as results of non-perturbation. Meanwhile, the susceptibility has been evaluated and the Shiba's relation has been exactly satisfied [29]. Taking all of these as the check and verification of the effectiveness of our analytical method, we further apply the method to study the current correlation function. The current correlation function

$$\begin{aligned} C(t) &= \frac{1}{2} \langle j(t)j(0) + j(0)j(t) \rangle \\ &= \frac{\Delta^2}{8} \langle \sigma_y(t)\sigma_y(0) + \sigma_y(0)\sigma_y(t) \rangle \end{aligned} \quad (23)$$

is defined as correlation of the tunneling current $j = \frac{1}{2}\Delta\sigma_y$ and its correlation time implies the lifetime of the coherent oscillations in the position correlation function $\langle\{\sigma_z(t), \sigma_z(0)\}\rangle$, therefore can predict correctly the coherent-incoherent transition [22].

To calculate the current correlation function, we take g_k as the perturbation parameter and use the Green's function method to implement the perturbation treatment. The retarded Green's function is defined as

$$\begin{aligned} G(t) &= -i\theta(t) \langle [\sigma_y(t), \sigma_y] \rangle \\ &= -i\theta(t) \langle [\sigma'_y(t), \sigma'_y] \rangle' \end{aligned} \quad (24)$$

where $\sigma'_i = e^S \sigma_i e^{-S}$, $\sigma'_i(t) = \exp(iH't) \sigma'_i \exp(-iH't)$, and $\langle \dots \rangle'$ means the average with thermodynamic probability $\exp(-\beta H')$. The Fourier transformation of $G(t)$ is denoted as $G(\omega)$ which satisfies an infinite chain of equation of motion [30]. By means of the cutoff approximation for the equation chain

$$\omega G(\omega) = \langle \langle [\sigma'_y(t), H'] | \sigma'_y \rangle \rangle'_\omega \quad (25)$$

at the second order of g_k , a set of equations is obtained:

$$\begin{aligned} \langle \langle [\sigma'_y(t), H'] | \sigma'_y \rangle \rangle'_\omega &= i\eta^2 \Delta \langle \langle \sigma_z(t) | \sigma'_y \rangle \rangle'_\omega \\ &+ i\eta \sum_k g_k \langle \langle \sigma_x(b_k^\dagger + b_k)(t) | \sigma'_y \rangle \rangle'_\omega \\ \omega \langle \langle \sigma_y(t) | \sigma'_y \rangle \rangle'_\omega &= i\eta \Delta \langle \langle \sigma_z(t) | \sigma'_y \rangle \rangle'_\omega \\ &+ i \sum_k V_k \langle \langle \sigma_x(b_k^\dagger + b_k)(t) | \sigma'_y \rangle \rangle'_\omega \\ \omega \langle \langle \sigma_z(t) | \sigma'_y \rangle \rangle'_\omega &= -2i\eta - i\eta \Delta \langle \langle \sigma_y(t) | \sigma'_y \rangle \rangle'_\omega \\ &- \sum_k V_k \langle \langle \sigma_x(b_k^\dagger - b_k)(t) | \sigma'_y \rangle \rangle'_\omega \\ \omega \langle \langle \sigma_x(b_k^\dagger - b_k)(t) | \sigma'_y \rangle \rangle'_\omega &= -V_k \langle \langle \sigma_z(t) | \sigma'_y \rangle \rangle'_\omega \\ &- \omega_k \langle \langle \sigma_x(b_k^\dagger + b_k)(t) | \sigma'_y \rangle \rangle'_\omega \\ \omega \langle \langle \sigma_x(b_k^\dagger + b_k)(t) | \sigma'_y \rangle \rangle'_\omega &= -2iV_k / \Delta \\ &- iV_k \langle \langle \sigma_y(t) | \sigma'_y \rangle \rangle'_\omega \\ &- \omega_k \langle \langle \sigma_x(b_k^\dagger - b_k)(t) | \sigma'_y \rangle \rangle'_\omega \end{aligned} \quad (26)$$

From this set of equations, the Green's function can be evaluated as:

$$\begin{aligned} G(\omega) &= \frac{\omega^2}{\Delta^2} \left(\frac{1}{\omega - \eta\Delta - \sum_k \frac{V_k^2}{\omega - \omega_k}} \right. \\ &\left. - \frac{1}{\omega + \eta\Delta - \sum_k \frac{V_k^2}{\omega + \omega_k}} \right) \end{aligned} \quad (27)$$

Thus the current correlation function:

$$\begin{aligned} C(t) &= -\frac{\Delta^2}{16\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \text{Im}G(\omega) \\ &= \frac{1}{4\pi} \int_0^{\infty} \frac{\omega^2 \gamma(\omega) \cos(\omega t)}{[\omega - \eta\Delta - R(\omega)]^2 + \gamma^2(\omega)} d\omega \end{aligned} \quad (28)$$

In evaluation of the integral the upper cutoff ω_c is used to determine the upper limit of the integration variable. According to property of Pauli matrices, $4C(t)/\Delta^2$ [see Eq. (23)] should be unity at initial time $t = 0$, which is well preserved by Eq. (28).

Figure 1 shows the current correlation function as function of the time $\Delta_r t$ in the cases of $\Delta_r/\omega_c = 0.01$ for different dampings $\alpha = 0.2, 0.3, 0.4$, and 0.5 . As shown in the figure, for finite renormalized tunneling the oscillatory behavior of the current correlation function can be clearly observed up to $\alpha = 0.5$, although its amplitude decreases rapidly with increasing of α , which illustrates that the coherent-incoherent transition point $\alpha_c > 1/2$ for $\Delta_r/\omega_c > 0$. For fixed value

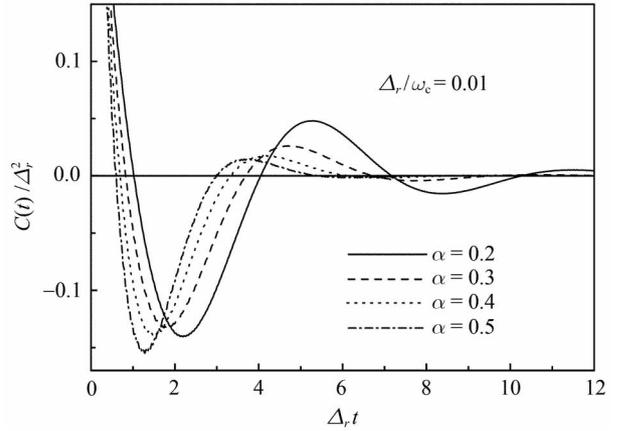


Fig. 1 The current correlation function as function of the time $\Delta_r t$ in the cases of $\Delta_r/\omega_c = 0.01$ for different dampings $\alpha = 0.2, 0.3, 0.4$, and 0.5 .

of the damping $\alpha = 0.5$, as the renormalized tunneling Δ_r declines the oscillatory behavior is weakened rapidly and finally disappears at the scaling limit $\Delta/\omega_c \ll 1$ at which the coherent-incoherent transition takes place. This process is plotted in Fig. 2. In this figure, to compare the change of

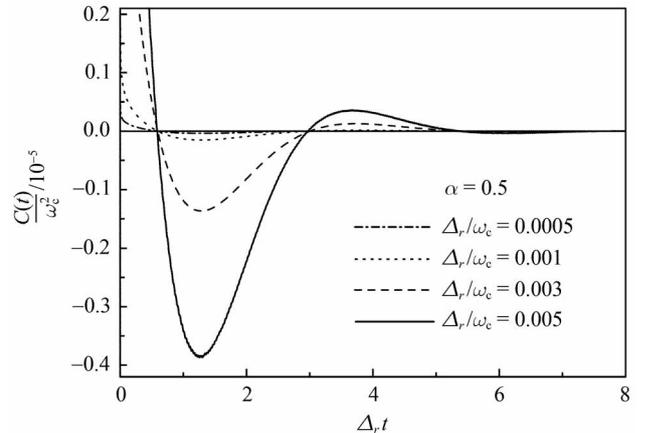


Fig. 2 The current correlation function as function of the time $\Delta_r t$ in the cases of $\alpha = 0.5$ for different renormalized tunneling $\Delta_r/\omega_c = 0.005, 0.003, 0.001$, and 0.0005 . For fixed damping $\alpha = 0.5$, the oscillatory behavior is weakened rapidly as the renormalized tunneling Δ_r declines and finally disappears at the scaling limit $\Delta/\omega_c \ll 1$.

the amplitude of the current correlation function for different Δ_r/ω_c , the current correlation function is scaled by ω_c^2 instead of renormalized tunneling as in Fig. 1. The comparisons of the coherent oscillation and the long-time decay of the current correlation function between numerical method [22] and our result in coherent phase are shown in Figs. 3 and 4. One can see that our results agree very well with that of numerical simulations [22] when $\alpha < \alpha_c$, which is important for our theory as a potential method to be applied to investigate the absorption spectra and photoluminescence in quantum dots and other confined quantum systems since in these systems the coupling constant α is usually small, though our method may be less accurate in incoherent phase of $\alpha > \alpha_c$ due to the cutoff approximation for the Heisenberg equation of motion and the choice of the coupling strength as the perturbation parameter in perturbation treatment. In comparison with results of numerical methods, in which the oscillatory behavior is

visible up to $\alpha \approx 0.4$ [19, 22] and the accuracy of numerical data does not allow one to resolve oscillatory behavior anymore after α passes that value [19], our theory can reveal the oscillatory behavior even for α very close to transition point α_c by virtue of the analytic expression of the current correlation function Eq. (28).

4 Summary

In summary, an analytical approach is developed to investigate the dynamic behavior of current correlation function of dissipative two-state systems with the view of understanding effects of environments and tunneling on the coherent oscillation and the long-time decay in these systems. An analytic expression of current correlation function is obtained and the results agree very well with that of numerical simulations in coherent phase. Our theory can be applied as a potential analytical method to investigate the absorption spectra and photoluminescence in quantum dots and other confined quantum systems.

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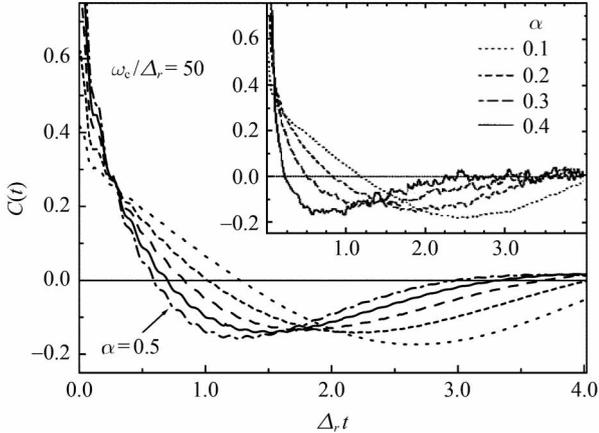


Fig. 3 The comparison of the coherent oscillations of the current correlation function in coherent phase between numerical method [22] and our result by using the same input parameters as in Ref. [22]. Inset: The result of numerical method from Ref. [22].

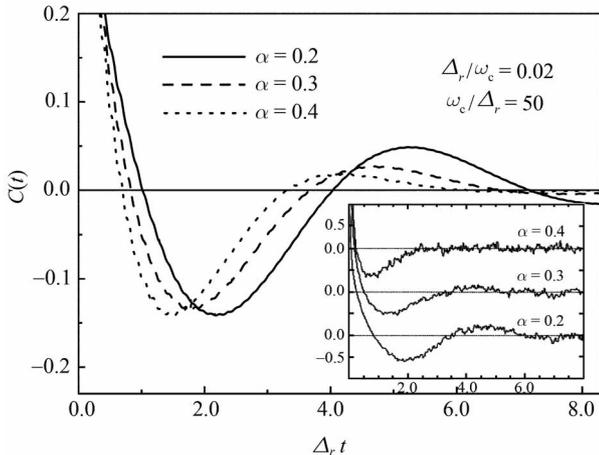


Fig. 4 The long-time decay of the current correlation function in coherent phase. Inset: The result of numerical method from Ref. [22].

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