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Dynamics of a two-level system coupled to Ohmic bath: a perturbation approach

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Abstract. The quantum dynamics, both non-equilibrium and equilibrium, of the dissipative two-level system is studied by means of the perturbation approach based on a unitary transformation. It works well for the whole parameter range $0 < \alpha < 1$ and $0 < \Delta < \omega_c$ and our main results are: the coherence-incoherence transition is at $\alpha_c = \frac{1}{2}[1 + \Delta_r/\omega_c]$; for $\alpha < \alpha_c$ the non-equilibrium correlation $P(t) = \cos(\omega_0 t)\exp(-\gamma t)$; the susceptibility $\chi''(\omega)/\omega$ is of a double peak structure for $\alpha < \alpha_c$ and the Shiba's relation is exactly satisfied; at the transition point $\alpha = \alpha_c$ the equilibrium correlation $C(t) \approx -1/\gamma_c^2 t^2$ in the long time limit.

PACS. 72.20.Dp General theory, scattering mechanisms – 05.30.-d Quantum statistical mechanics

Quantum dynamics in the two-level system coupled to Ohmic bath (spin-boson model, SBM) is important to understand numerous physical and chemical processes since it provides a universal model for these processes [1,2], such as the defect-tunneling in solids and the macroscopic quantum coherence experiment in SQUID's. The Hamiltonian of SBM reads

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

The notations are the same as usual [1,2]. In this work we consider the zero bias case with temperature $T = 0$. The Ohmic bath is characterized by its spectral density: $\sum_k g_k^2\delta(\omega-\omega_k) = 2\alpha\omega\theta(\omega_c-\omega)$, where α is the dimensionless coupling constant and $\theta(x)$ is the usual step function.

The Hamiltonian (1) seems quite simple. However, it cannot be solved exactly and various approximate analytical and numerical methods have been used [1–13]. The main theoretical interest is to understand how the environment influences the dynamics of the two-level system and, in particular, how dissipation destroys quantum coherence. Both the non-equilibrium and equilibrium dynamics are of interest for the different experimental realizations of two-level systems. When the system can be prepared in one of the two states by applying a bias for times $t < 0$ and then let it evolve for $t > 0$ in zero bias, the non-equilibrium correlation function $P(t)$ is of primary interest [1,6]. When the initial state preparation is not realizable, the interest is then lies in the equilibrium correlation function $C(t)$ and the susceptibility $\chi(\omega)$ [2–4,7–9]. Moreover, the real and imaginary parts of $\chi(\omega)$ should satisfy the Shiba's relation [3,7,9,12]. As far as we know, there is no single analytical or numerical approach which can produce correct behavior of $P(t)$, $C(t)$, and $\chi(\omega)$ for the whole parameter range $0 < \alpha < 1$ and $0 < \Delta < \omega_c$.

In this work we present a new analytical approach, based on the unitary transformation method and the perturbation theory [14], for calculating both the non-equilibrium and equilibrium dynamics of SBM. It works well for the coupling constant $0 < \alpha < 1$ and the bare tunneling $0 < \Delta < \omega_c$, and can reproduce nearly all results of previous authors (they used various analytical and numerical methods). The approach is quite simple and physically clear, and may be easily extended to more complicated coupling systems.

Silbey and Harris [13] proposed to make a unitary transformation to H: $H' = \exp(S)H\exp(-S)$,

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

The variational ground state energy is supposed to be: $E_g = \langle s_1|\langle\{0_k\}|H'|s_1\rangle|\{0_k\}\rangle$, where $|s_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ and $|s_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$ are eigenstates of σ_x and $|\{0_k\}\rangle$ is the vacuum state of bosons in which $n_k = 0$ for every k. By minimizing E_g, ξ_k is determined as

$$\xi_k = \omega_k/(\omega_k + \eta\Delta). \quad (3)$$

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The authors calculated the renormalized tunneling Δ_r [13],

$$\eta = \frac{\Delta_r}{\Delta} = \left(e\frac{\Delta}{\omega_c}\right)^{\frac{\alpha}{1-\alpha}} \exp\left[-\frac{\alpha}{1-\alpha}\left(\frac{\eta\Delta}{\omega_c+\eta\Delta} + \ln\frac{\omega_c+\eta\Delta}{\omega_c}\right)\right]. \tag{4}$$

Although the variational method can predict correctly the delocalized-localized transition point $\alpha_l = 1$ at the scaling limit $\Delta/\omega_c \ll 1$, it is not suitable for calculating the dynamical properties of SBM.

A method of unitary transformation plus perturbation calculation was used by Aslangul et al. [15] and by Dekker [16] to treat the same problem. But their unitary transformation is different from that in (2) (if $\xi_k = 1$ in transformation Eq. (2), then it is the same as theirs). Their perturbation treatment is good only for the scaling limit $\Delta/\omega_c \ll 1$. Besides, Kehrein et al. [17] used the continuous infinitesimal unitary transformations to diagonalize H (Eq. (1)) step by step and some static properties of SBM were correctly predicted, such as the untraped-traped transition at $\alpha = \alpha_l = 1$ (when $\Delta/\omega_c \ll 1$). However, it seems difficult to calculate dynamical properties of SBM, especially the non-equilibrium correlation $P(t)$ [1,6], by the approach of Kehrein et al. They dealt with a transition from coherent to incoherent tunneling at some finite temperature T_2^*, but they did not treat the zero temperature coherent-incoherent transition at $\alpha = \alpha_c$.

Our approach starts from the unitary transformation (2) and then make perturbation calculation for the transformed Hamiltonian. The transformation can be done to the end and the result is $H' = H'_0 + H'_1 + H'_2$, where

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

$$\eta = \exp\left[-\sum_k \frac{g_k^2}{2\omega_k^2}\xi_k^2\right], \tag{6}$$

$$H'_1 = \frac{1}{2}\sum_k g_k(1-\xi_k)(b_k^\dagger + b_k)\sigma_z - \frac{1}{2}\eta\Delta i\sigma_y \sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k), \tag{7}$$

$$H'_2 = -\frac{1}{2}\Delta\sigma_x\left(\cosh\left\{\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\right\} - \eta\right) - \frac{1}{2}\Delta i\sigma_y\left(\sinh\left\{\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\right\} - \eta\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\right). \tag{8}$$

Obviously, H'_0 can be solved exactly because in which the spin and bosons are decoupled. The eigenstate of H'_0 is a direct product, $|s\rangle|\{n_k\}\rangle$, where $|s\rangle$ is $|s_1\rangle$ or $|s_2\rangle$ and $|\{n_k\}\rangle$ means that there are n_k phonons for mode k. The ground state of H'_0 is

$$|g_0\rangle = |s_1\rangle|\{0_k\}\rangle. \tag{9}$$

H'_1 and H'_2 are treated as perturbation and they should be as small as possible. Equation (3), $\xi_k = \omega_k/(\omega_k + \eta\Delta)$, leads to

$$H'_1 = \frac{1}{2}\eta\Delta\sum_k \frac{g_k}{\omega_k}\xi_k\left[b_k^\dagger(\sigma_z - i\sigma_y) + b_k(\sigma_z + i\sigma_y)\right] \tag{10}$$

and $H'_1|g_0\rangle = 0$. Note that the form of ξ_k, equation (3), in this work is determined by $H'_1|g_0\rangle = 0$, instead of minimizing the ground state energy E_g. Thus, we get rid of the variational condition.

The lowest excited states are $|s_2\rangle|\{0_k\}\rangle$ and $|s_1\rangle|1_k\rangle$, where $|1_k\rangle$ is the number state with $n_k = 1$ but $n_{k'} = 0$ for all $k' \neq k$. It's easily to check that $\langle g_0|H'_2|g_0\rangle = 0$ (because of the form of η in Eq. (6)), $\langle\{0_k\}|\langle s_2|H'_2|g_0\rangle = 0$, $\langle 1_k|\langle s_1|H'_2|g_0\rangle = 0$, and $\langle\{0_k\}|\langle s_2|H'_2|s_1\rangle|1_k\rangle = 0$. Moreover, since $H'_1|g_0\rangle = 0$, we have $\langle\{0_k\}|\langle s_2|H'_1|g_0\rangle = 0$ and $\langle 1_k|\langle s_1|H'_1|g_0\rangle = 0$. Thus, we can diagonalize the lowest excited states of H' as

$$H' = -\frac{1}{2}\eta\Delta|g_0\rangle\langle g_0| + \sum_E E|E\rangle\langle E| + \text{terms with higher excited states}. \tag{11}$$

The diagonalization is through the following transformation [4]:

$$|s_2\rangle|\{0_k\}\rangle = \sum_E x(E)|E\rangle, \tag{12}$$

$$|s_1\rangle|1_k\rangle = \sum_E y_k(E)|E\rangle, \tag{13}$$

$$|E\rangle = x(E)|s_2\rangle|\{0_k\}\rangle + \sum_k y_k(E)|s_1\rangle|1_k\rangle, \tag{14}$$

where

$$x(E) = \left[1 + \sum_k \frac{V_k^2}{(E + \eta\Delta/2 - \omega_k)^2}\right]^{-1/2}, \tag{15}$$

$$y_k(E) = \frac{V_k}{E + \eta\Delta/2 - \omega_k}x(E), \tag{16}$$

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

$$E - \frac{\eta\Delta}{2} - \sum_k \frac{V_k^2}{E + \eta\Delta/2 - \omega_k} = 0. \tag{17}$$

The non-equilibrium correlation $P(t) = \langle b,+1|\langle +1|e^{iHt}\sigma_z e^{-iHt}|+1\rangle|b,+1\rangle$ is defined in reference [1], where $|+1\rangle$ is the eigenstate of $\sigma_z = +1$ and $|b,+1\rangle$ is the state of bosons adjusted to the state of $\sigma_z = +1$. Because of the unitary transformation ($e^S\sigma_z e^{-S} = \sigma_z$)

$$P(t) = \langle\{0_k\}|\langle +1|e^{iH't}\sigma_z e^{-iH't}|+1\rangle|\{0_k\}\rangle, \tag{18}$$

since $e^S|+1\rangle|b,+1\rangle = |+1\rangle|\{0_k\}\rangle$. Using equations (11–17) the result is

$$\begin{aligned} P(t) &= \frac{1}{2}\sum_E x^2(E)\exp[-i(E+\eta\Delta/2)t] \\ &\quad + \frac{1}{2}\sum_E x^2(E)\exp[i(E+\eta\Delta/2)t] \\ &= \frac{1}{4\pi i}\oint_C dE' e^{-iE't}\left(E'-\eta\Delta-\sum_k\frac{V_k^2}{E'+i0^+-\omega_k}\right)^{-1} \\ &\quad + \frac{1}{4\pi i}\oint'_C dE' e^{iE't}\left(E'-\eta\Delta-\sum_k\frac{V_k^2}{E'-i0^+-\omega_k}\right)^{-1}, \end{aligned} \quad (19)$$

where a change of the variable $E' = E + \eta\Delta/2$ is made. The real and imaginary parts of $\sum_k V_k^2/(E' \pm i0^+ - \omega_k)$ are denoted as $R(E')$ and $\mp\gamma(E')$,

$$R(\omega) = -2\alpha\frac{(\eta\Delta)^2}{\omega+\eta\Delta}\left\{\frac{\omega_c}{\omega_c+\eta\Delta} - \frac{\omega}{\omega+\eta\Delta}\ln\left[\frac{|\omega|(\omega_c+\eta\Delta)}{\eta\Delta(\omega_c-\omega)}\right]\right\}, \quad (20)$$

$$\gamma(\omega) = 2\alpha\pi\omega(\eta\Delta)^2/(\omega+\eta\Delta)^2. \quad (21)$$

The integral in (19) can proceed by calculating the residue of integrand and the result is $P(t) = \cos(\omega_0 t)\exp(-\gamma t)$, where ω_0 is the solution of equation

$$\omega - \eta\Delta - R(\omega) = 0 \quad (22)$$

and $\gamma = \gamma(\eta\Delta) = \alpha\pi\eta\Delta/2$ (the second order approximation). This $P(t)$ is of the form of damped oscillation and one can check that the solution ω_0 is real when $1 > 2\alpha\omega_c/(\omega_c+\eta\Delta)$. When $1 < 2\alpha\omega_c/(\omega_c+\eta\Delta)$, the solution ω_0 is imaginary and we have an incoherent $P(t)$. $\alpha_c = \frac{1}{2}[1+\eta\Delta/\omega_c]$ determines the critical point where there is a coherent-incoherent transition. Note that when $\Delta/\omega_c \ll 1$ and $\alpha = \alpha_c = 1/2$, we have $\omega_0 = 0$ and $P(t) = \exp(-\gamma_c t)$ ($\gamma_c = \pi e\Delta^2/4\omega_c$ since $\eta = e\Delta/\omega_c$ from Eq. (4)), which is the same as was predicted by previous authors ($\gamma_c = \pi\Delta^2/2\omega_c$ in Refs. [3,4,6]). Figure 1 shows the calculated ω_0/Δ_r as functions of α ($\alpha \le \alpha_c$) for $\Delta = 0.01$, 0.1, and 0.5. $\Delta_r = \eta\Delta$ is the renormalized tunneling. The dotted line is $\gamma/\Delta_r = \alpha\pi/2$.

The coherent-incoherent transition point $\alpha_c = \frac{1}{2}[1+\eta\Delta/\omega_c]$ increases with increasing Δ/ω_c. Only at the scaling limit $\Delta/\omega_c \ll 1$ does α_c take the value $\alpha_c = \frac{1}{2}$. This result seems to be deviated from the equivalence between SBM and the fermionic resonant level model (RLM), since the latter predicts $\alpha_c = \frac{1}{2}$. We believe that the deviation comes from the approximation introduced when the bosonization technique is used to map SBM to RLM [4]. As was pointed out in reference [4], the equivalence between SBM and RLM is regolous only in the limit where the momentum cutoff $1/a$ goes to infinity, which is equivalent to $\omega_c \to \infty$ in this work. This is to say that, away from the scaling limit and when $0 < \Delta < \omega_c$, the equivalence between SBM and RLM is approximately and one can expect some deviation of the properties of SBM from those of RLM.

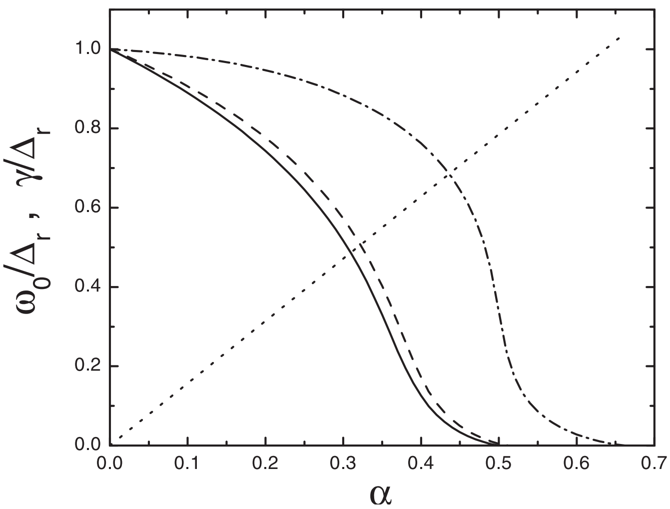

Fig. 1. $S(\omega)$ as functions of ω for fixed $\alpha = 0.3$ and $\Delta = 0.01$ (solid line), 0.1 (dashed), and 0.5 (dashed-dotted). The dotted line is $\gamma/\Delta_r = \alpha\pi/2$.

Since $e^S\sigma_z e^{-S} = \sigma_z$, the retarded Green's function is

$$G(t) = -i\theta(t)\left\langle[\exp(iH't)\sigma_z\exp(-iH't),\sigma_z]\right\rangle', \quad (23)$$

where $\langle ...\rangle'$ 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 [18]. We have made the cutoff approximation for the equation chain at the second order of g_k and the solution at $T = 0$ is

$$G(\omega) = \frac{1}{\omega-\eta\Delta-\sum_k V_k^2/(\omega-\omega_k)} - \frac{1}{\omega+\eta\Delta-\sum_k V_k^2/(\omega+\omega_k)}. \quad (24)$$

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

$$\chi''(\omega) = \frac{\gamma(\omega)\theta(\omega)}{[\omega-\eta\Delta-R(\omega)]^2+\gamma^2(\omega)} - \frac{\gamma(-\omega)\theta(-\omega)}{[\omega+\eta\Delta+R(-\omega)]^2+\gamma^2(-\omega)}. \quad (25)$$

The $\omega \to 0$ limit of $S(\omega) = \chi''(\omega)/\omega$ is

$$\lim_{\omega\to 0}\frac{\chi''(\omega)}{\omega} = \frac{2\alpha\pi}{(\eta\Delta)^2\{1-2\alpha[1-\eta\Delta/(\omega_c+\eta\Delta)]\}^2}. \quad (26)$$

Besides, the real part of the susceptibility is

$$\chi'(\omega=0) = \frac{2}{\eta\Delta\{1-2\alpha[1-\eta\Delta/(\omega_c+\eta\Delta)]\}}. \quad (27)$$

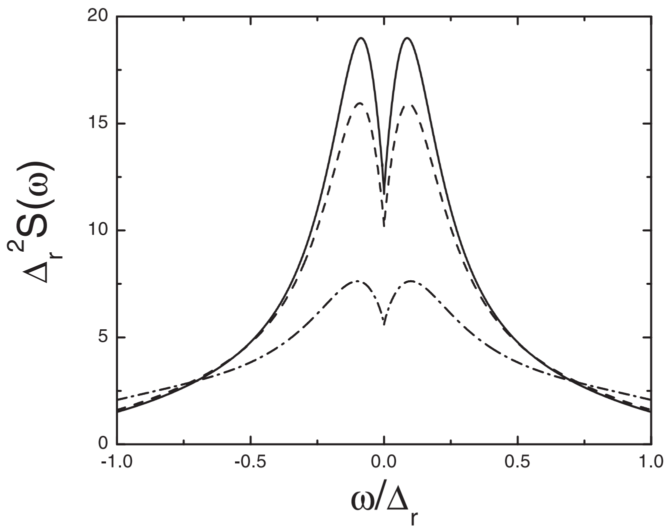

Fig. 2. ω_0/Δ_r versus α relations for $\Delta/\omega_c = 0.01$ (solid line, $\alpha_c = 0.50014$), 0.1 (dashed, $\alpha_c = 0.51212$), and 0.5 (dashed-dotted, $\alpha_c = 0.66244$).

Thus, the Shiba's relation [3,7,9,12]

$$\lim_{\omega\to 0} \frac{\chi''(\omega)}{\omega} = \frac{\pi}{2}\alpha\chi'(\omega = 0)^2 \tag{28}$$

is exactly satisfied. $S(\omega)$ has a double peak structure for $\alpha < \alpha_c$. For $\alpha \geq \alpha_c$ there is only one peak at $\omega = 0$. Figure 2 shows the $S(\omega)$ versus ω relations for fixed $\alpha = 0.3$ and $\Delta = 0.01$, 0.1, and 0.5.

The equilibrium correlation

$$\begin{aligned} C(t) &= \frac{1}{2}\mathrm{Tr}\big\{ \exp(-\beta H)[\sigma_z(t)\sigma_z \\ &\quad + \sigma_z\sigma_z(t)]\big\}/\mathrm{Tr}[\exp(-\beta H)] \\ &= -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \coth\left(\frac{\beta\omega}{2}\right) \mathrm{Im}G(\omega)\exp(-i\omega t) \\ &= \frac{1}{\pi}\int_0^{\infty} d\omega \frac{\gamma(\omega)}{[\omega - \eta\Delta - R(\omega_0)]^2 + \gamma^2}\cos(\omega t), \end{aligned} \tag{29}$$

where ω_0 is the solution of equation (22) and $\gamma(\omega)$ in the denominator is approximated by the second order approximation γ. For general value of $\alpha \leq \alpha_c$, $C(t)$ may contain both terms of the exponential decay ones and the algebraic decay ones. In the long-time limit the first non-zero algebraic decay term dominates which is $\sim -1/t^2$. For the special point $\alpha = \alpha_c$ ($\omega_0 = 0$), the exponential decay terms disappear. At the scaling limit $\Delta/\omega_c \ll 1$ and the coherence-incoherence transition point $\alpha = 1/2$,

$$C(t) = \int_0^{\infty} d\omega \frac{\omega\cos(\omega t)}{\omega^2 + \gamma_c^2}\frac{(\eta\Delta)^2}{(\omega + \eta\Delta)^2}. \tag{30}$$

$C(t)$ decays algebraically in the long-time limit: $C(t) \approx -1/\gamma_c^2 t^2$, which is the same as what was predicted by previous authors [2,3,6].

In summary: the dynamics of SBM is studied by means of the perturbation approach based on a unitary transformation. Analytical results of the non-equilibrium correlation $P(t)$, the susceptibility $\chi''(\omega)$ and the equilibrium correlation $C(t)$ are obtained for both the scaling limit $\Delta_r/\omega_c \ll 1$ and the general finite Δ_r/ω_c case. Our approach is quite simple, but it can reproduce nearly all results which agree with those of previous authors using various complicated methods. Besides, our approach can be easily extended to other more complicated coupling systems.

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