Decoherence and relaxation of qubits coupled to low- and medium-frequency Ohmic baths directly and via a harmonic oscillator

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Abstract

Using the numerical path integral method we investigate the decoherence and relaxation of qubits in spin-boson (SB) and spin-intermediate harmonic oscillator (IHO)-bath (SIB) models. The cases that the environment baths with low and medium frequencies are investigated. It is shown that the qubits in SB and SIB models have the same decoherence and relaxation as the baths with low frequencies. However, the qubits in the two models have different decoherence and relaxation as the baths with medium frequencies. The decoherence and relaxation of the qubit in SIB model can be modulated through changing the coupling coefficients of the qubit-IHO and IHO-bath and the oscillation frequency of the IHO.

Keywords: Decoherence; relaxation; path integral; spin-boson.

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I. INTRODUCTION

A two-level system, namely a qubit in today’s modern physical language is a most simple quantum physical model. If we only consider a closed qubit its dynamics is simple enough and has been well known. However, in fact, there is not any system being separated from its environment, in nature. The interaction between the qubit and its environment should be considered when we investigate the qubit’s dynamics. The interaction make the open qubit model become very complex and it may not be solved analytically exactly. In order to investigate the model, in most cases, the environment is modeled with a thermal bath which is considered being constructed with a set of harmonic oscillators. A typical open qubit model is the well known spin-boson (SB) model [1, 2, 3]. There is another open qubit model in which the qubit couples to the coordinate $X$ of a harmonic oscillator which we shall sometimes call the “intermediate harmonic oscillator” (IHO) and which in turn is coupled to a bath [4, 5, 6]. We call the model the spin-IHO-bath (SIB) model.

It has be found that the two models have many physical correspondences. In recent years the investigations of the two models have attached great interest of scientists in fields of quantum information, electron transfer, etc. [7, 8, 9, 10, 11, 12, 13, 14]. These are motivated by two exciting challenges, quantum computation and solar energy utilization. It is believed that quantum computers may perform some useful tasks more efficiently than their classical counterparts. Despite the great promises of performing quantum computations, however, there are still many practical difficulties to be resolved before quantum computers might become available in future. One of the difficulties is that the qubit has too short decoherence time, which is in fact a central impediment for practical solid-state qubits to be taken as the cell of quantum computers. Many significant results in the field, not only theoretical but also experimental, have been achieved. Most of the theoretical research is based on the SB and SIB models. On the other hand, the SB and SIB models can be used to describe the electron transfer in chemical and biological molecules. It has been recent found that the coherence is very important to electrons for transferring energy in biological systems [15, 16]. So it is important to investigate the decoherence and the relaxation of the electron spin (qubit).

In order to investigate the decoherence and relaxation of qubit in SB and SIB models, essentially, one must understand the dynamics of the qubit [17, 18, 19]. If the qubit energy splitting (denoted by $\Delta$ hereinafter) is not equal to zero, the two models are not exactly solvable. However, they can be analyzed using adiabatic renormalization in which a systematic weak damping approximation must be used. They can also be investigated with some approximation methods based on the perturbative scheme which also asks for the system (qubit) weakly coupling to its environment. Many other methods [20, 21, 22, 23, 24, 25] for solving the models have been proposed in recent years, most of which are based on the Born-Markov approximation. However, it has been pointed out that the use of the approximation is inappropriate at the large tunneling amplitude and low temperatures. So it is important to find out some methods to accurately estimate the dynamics of the qubits in the two models. Based on the insight into the dynamics we may understand the decoherence and relaxation better and may bring forward some schemes on how to suppress them. An excellent, accurate numerical method based on the quasiadiabatic propagator path integral (QUAPI) [26, 27] may be a suitable tool for solving the two models. To our problems we choose the iterative tensor multiplication (ITM) algorithm for the numerical scheme. As Makri [26, 27] addressed that the method is non-Markovian and it can make the calculations accurate enough even at very low temperatures, large tunneling amplitudes and strong couplings for which the Markovian
II. MODELS AND DYNAMICS

The Hamiltonian of the SB model is

\[ H_{SB} = \frac{\hbar}{2}(\sigma_x + \Delta \sigma_x) + \sum_i \left[ \frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2 \left( x_i + \frac{c_i\sigma_z}{m_i\omega_i^2} \right)^2 \right] \]

Suppose the bath has an Ohmic spectral density

\[ J_{ohm}(\omega) = \frac{\pi}{2} \sum_i \frac{c_i^2}{m_i\omega_i}\delta(\omega - \omega_i) = \frac{\pi}{2}\eta\omega e^{-\omega/\omega_c}. \] (1)

Here, \( \xi \) is the dimensionless Kondo parameter \( 10, 20 \) (the relationship of \( \xi \) with the friction coefficient \( \eta \) is \( \xi = 2\eta/\pi\hbar \) [31]), \( \sigma_i \) (\( i = x, z \)) are the Pauli matrix, and \( \omega_c \) is the high-frequency cut-off of the bath modes. This is a well-known quantum dissipation model and it has been widely investigated \( 1, 2 \).

If we consider the qubit coupling to the coordinate \( X \) of a single IHO which in turn is coupled to a bath, and if we let the couplings be linear, the Hamiltonian of the SIB system reads

\[ H_{SIB} = \frac{\hbar}{2}(\sigma_z + \Delta \sigma_z) + \sum_i \left[ \frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2 \left( x_i + \frac{\kappa c_i X}{m_i\omega_i^2} \right)^2 \right] + \sum_i \left[ \frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2 \left( \tilde{x}_i + \frac{\kappa c_i X}{m_i\omega_i^2} \right)^2 \right], \] (2)

where \( M \) and \( P \) are the mass and momentum of the IHO, and the displacement \( \lambda \) characterizes the coupling of the qubit to the IHO, and \( \kappa c_i \) are the coupling coefficients of the IHO to the bath modes. It is shown that the system has a one to one map to the following system [4]

\[ H_{SIB} = \frac{\hbar}{2}(\sigma_x + \Delta \sigma_x) + \sum_i \left[ \frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2 \left( \tilde{x}_i + \frac{\delta c_i}{m_i\omega_i^2} \right)^2 \right]. \] (3)

According to paper I, as the high-frequency cut-off of the bath mode is not infinite the effective spectral density is

\[ J_{eff}(\omega) = \frac{\pi}{2} \sum_i \frac{c_i^2}{m_i\omega_i}\delta(\omega - \omega_i) = \frac{\pi}{2}\eta\omega e^{-\omega/\omega_c}. \]

where \( \Gamma = \kappa^2\eta/2M \). The spectral density functions of \( J_{ohm}(\omega) \) and \( J_{eff}(\omega) \) versus bath modes' frequencies are plotted in Fig. 1.

![Fig. 1](image1)

Fig. 1: The spectral density functions \( J_{ohm}(\omega) \) and \( J_{eff}(\omega) \) versus the frequency \( \omega \) of the bath modes, where \( \Delta = 5 \times 10^9 \) Hz, \( \lambda\kappa = 1 \), \( \xi = 0.01 \), \( \Omega_0 = 10\Delta \), \( T = 0.01 \) K, \( \Gamma = 2.6 \times 10^{11} \) Hz.

Here, we set \( \lambda\kappa = 1 \) and other parameters are same as in paper I, namely, \( \Delta = 5 \times 10^9 \) Hz, \( \xi = 0.01 \), \( \Omega_0 = 10\Delta \), \( T = 0.01 \) K, \( \Gamma = 2.6 \times 10^{11} \) Hz. From Fig.1 we see that the spectral density functions have following characteristics. When the frequencies of the bath modes are low (\( 0 < \omega < 0.1\Delta \)) the \( J_{ohm}(\omega) \) and \( J_{eff}(\omega) \) increase linearly with the bath frequency \( \omega \) and they are equivalent, see Fig. 1. When the frequencies of the bath modes are medium (\( 0.1\Delta < \omega \leq 1\Delta \)) the \( J_{ohm}(\omega) \) and \( J_{eff}(\omega) \) behave in their different ways, see the insetted figures in Fig. 1. In particular, in the model SIB, the IHO resonate with some mode of the bath within the frequency limits. When the frequencies of the bath modes are high (\( 1\Delta < \omega \leq 100\Delta \)) the \( J_{ohm}(\omega) \) and \( J_{eff}(\omega) \) decrease with the bath frequency \( \omega \). We call the bath modes with low- \( (0 < \omega < 0.1\Delta) \), medium- \( (0.1\Delta < \omega < 1\Delta) \) and high-frequency \( (1\Delta < \omega \leq 100\Delta) \) the low-, medium- and high-frequency baths respectively. The range of frequencies for the low-, medium- and high-frequency baths are plotted in Fig. 2 and they are represented with Low F, Medium F and High F in the figure.

![Fig. 2](image2)

Fig. 2: The sketch map on the low-, medium-, and high-frequency baths.

When the bath modes have high frequencies the dynamics of the qubit in SB and SIB models has been investigated in paper I. In this paper we investigate other two cases, namely, the cases of low- and medium-frequency baths. The IHO is resonance with one of the modes of the medium-frequency bath. The length of the memory
times of the baths can be estimated by the following bath response function

$$\alpha(t) = \frac{1}{\pi} \int_0^\infty d\omega J(\omega) \left[ \coth \left( \frac{\beta \hbar \omega}{2} \right) \cos \omega t - i \sin \omega t \right].$$

Here, $\beta = 1/k_B T$ where $k_B$ is the Boltzmann constant, and $T$ is the temperature. It is shown that when the real and imaginary parts behave as the delta function $\delta(t)$ and its derivative $\delta'(t)$, the dynamics of the reduced density matrix is Markovian. However, if the real and imaginary parts are broader than the delta function, the dynamics is non-Markovian. The broader the the real or imaginary parts, the longer the memory time will be. The broader the Re$[\alpha(t)]$ and Im$[\alpha(t)]$ are, the more serious the practical dynamics will be distorted by the Markovian approximation. The memory time of the effective bath is affected by $\Gamma$. The larger the $\Gamma$ is, the shorter the memory time of the effective bath will be. Clearly, the value of the $\Gamma$ may be different according to the difference of the physical systems. For example, when the persistent-current qubit is measured by a dc SQUID, the system can be modeled by Eq. (4) with Eq. (5), here $\Gamma = 1/R_C s$. Typically, $R_C = 100 \Omega$, $C_s = 5 \text{ pF}$, so $\Gamma \sim 10^{11} \text{ Hz}$, see Ref. 32. Similar to paper I we set $\Gamma = 2.6 \times 10^{11} \text{ Hz}$ in this paper. In Fig. 3 we plot the Re$[\alpha(t)]$ and Im$[\alpha(t)]$ of the low-frequency bath as (a) $J(\omega) = J_{\text{ohm}}(\omega)$, and (b) $J(\omega) = J_{\text{eff}}(\omega)$ and the medium-frequency bath as (c) $J(\omega) = J_{\text{ohm}}(\omega)$, and (d) $J(\omega) = J_{\text{eff}}(\omega)$. It is shown that the memory times in above four cases are all about $\tau_m \approx 1.5/\Delta$.

Fig. 3: The response functions of the Ohmic bath in (a) low and (c) medium frequencies and effective bath in (b) low and (d) medium frequencies. The parameters are the same as in Fig. 1. The cut-off frequencies for the two cases are taken according to Fig. 2.

The dynamics of the qubit is characterized by the time evolution of the reduced density matrix, obtained after tracing out the bath degrees of freedom, i.e.,

$$\rho(s'' \rightarrow s', t) = \text{Tr}_{\text{bath}} \langle s'' | e^{-i\mathcal{H}t/\hbar} R(0) e^{i\mathcal{H}t/\hbar} | s' \rangle. \quad (7)$$

Throughout this paper we assume that the interaction between system and bath is turned on at $t = 0$, such that the initial density matrix factorizes into its system and bath components, and the bath is initially at thermal equilibrium $[24, 31]:$

$$R(0) = \rho(0) \otimes \rho_{\text{bath}}(0), \quad (8)$$

where $\rho(0)$ and $\rho_{\text{bath}}(0)$ are the initial states of the qubit and bath. Here, we calculate the reduced density matrix $\rho(t)$ by using the well established ITM algorithm derived from the QUAPI. This algorithm is a numerically exact one and is successfully tested and adopted in various problems of open quantum systems [10, 23, 30]. For details of the scheme, we refer to previous works [26, 27]. The QUAPI asks for the system Hamiltonian splitting into two parts $H_0$ and $H_{\text{env}}.$ Here, we take $H_0 = \hbar \omega_x (\sigma_x + \Delta \sigma_z)$ and $H_{\text{env}} = H_{SB} - H_0$, or $H_{\text{env}} = H_{SIB} - H_0$. In order to make the calculations converge we use the time step $\Delta t = 0.5/\Delta$, which is smaller than the characteristic times of the qubits in the systems.

III. DECOHERENCE AND RELAXATION

The decoherence is in general produced due to the interaction of the quantum system with other systems with a large number of degrees of freedom, for example the devices of the measurement or environment. To measure the decoherence one may use the entropy, the first entropy, and many other measures, such as the maximal deviation norm, etc. (see for example Refs. 33, 34). However, essentially, the decoherence of an open quantum system is reflected through the decays of the off-diagonal coherent terms of its reduced density matrix [23]. The decoherence time denoted by $\tau_2$ measures the time of the initial coherent terms to their $1/e$ times, namely, $\rho_i(n, m) \approx \rho_i(n, m)/e$. Here, $n \neq m$, and $n, m = 0$ or 1 for qubits. In the following, we investigate the decoherence of the qubit in SB and SIB models via directly calculating the evolutions of the off-diagonal coherent terms, instead of some measure of the decoherence. Similar to the decoherence, the relaxation of the qubit can also be investigated with calculating the evolutions of the diagonal elements of the reduced density matrix. The relaxation time is denoted by $\tau_1$, which measures the time of an initial state to the final thermal equilibrium state through estimating the diagonal terms of the reduced density matrix, namely, $\rho_i(n, m) \approx e^{-E_n/\beta}$. In the following calculations we assume that the initial state of the environment is $\rho_{\text{bath}}(0) = \prod_k e^{-\beta M_k}/\text{Tr} \{ e^{-\beta M_k} \}$ and initially the qubit in its maximal coherent state. Here, $M_k = \hbar \omega_k b_k^\dagger b_k$ where $b_k^\dagger (b_k)$ are the create (annihilate) operators of the $k$-th mode for the environment. As calculating the off-diagonal element $\rho_{12}$ we let $\epsilon = 10\Delta$ which can make the $\rho_{12}$ decay stably. If $\epsilon \rightarrow \Delta$ the $\rho_{12}$ will decay with some oscillations, which may affect our judgement on decoherence times. The closer the two parameters are, the more strongly the matrix elements will oscillate. When we calculate $\rho_{11}$ we choose parameters $\epsilon = \Delta$ because the oscillations of the $\rho_{11}$ do not affect our judgement on relaxation times from the figures. If we choose parameters $\epsilon = 10\Delta$ other than $\epsilon = \Delta$ in calculating the $\rho_{11}$, the relaxation of the qubit cannot be shown clearly in the figures in a short time because the time $\tau_1$ is greatly larger than the time $\tau_2$ in our problems. So, the reader should note that, the increase of the $\Delta$ and $\epsilon$ will shorten the decoherence and relaxation times,
the decoherence time $\tau_2$ and the relaxation time $\tau_1$ in following figures are not comparable because they are plotted in different two sets of the parameters. In the ITM scheme, one should at first choose the $k_{\text{max}}$ and assure that $k_{\text{max}}\Delta t$ is larger than the effective memory time $\tau^m$ of the baths. Fig. 3 and numerical tests tell us that the calculations are in fact convergent as $k_{\text{max}} \geq 3$. It is known that the qubit will show different decoherence and relaxation when it has different initial states. In the low- and medium-frequency baths, the decoherence and relaxation of the qubits in their different initial states are different, which is similar to the cases of high-frequency bath (see Fig. 3 of paper I), we do not plot the evolutions of $\rho_{12}$ and $\rho_{11}$ in different initial states in this paper. Fig. 4 plots the evolutions of the $\rho_{12}$ (below) and $\rho_{11}$ (up) of the qubit in low-frequency bath in SB and SIB models. It is shown that the qubit in SB and SIB models has almost same decoherence and relaxation in this case.

**Fig.4**

Fig. 4: The evolutions of reduced density matrix elements $\rho_{12}$ (below) and $\rho_{11}$ (up) in SB and SIB models in low-frequency bath. The parameters are the same as in Fig. 1.

**Fig.5**

Fig. 5: The evolutions of reduced density matrix elements of $\rho_{12}$ (below) and $\rho_{11}$ (up) in SB and SIB models in the medium-frequency bath ($\lambda\kappa = 1$, or 1.125). The other parameters are the same as in Fig. 1.

**Fig.6**

Fig. 6: The evolutions of reduced density matrix elements of $\rho_{12}$ (below) and $\rho_{11}$ (up) in SIB model in medium-frequency bath in different values of $\Omega_0$, the other parameters are the same as in Fig. 1.

Fig. 5 plots the evolutions of the $\rho_{12}$ (below) and $\rho_{11}$ (up) of the qubit in medium-frequency bath in SB and SIB models. It is shown that as $\kappa\lambda = 1$, the qubit in SIB model has longer decoherence and relaxation times than the qubit in SB model has. As $\kappa\lambda$ increase to 1.125 the qubit in SIB model has almost same decoherence and relaxation times to the qubit in SB model has, but the $\rho_{11}$ decays to a bigger equilibrium value. Fig. 6 plots the $\rho_{12}$ (below) and $\rho_{11}$ (up) of the qubit in SIB model in different $\Omega_0$ of the IHO in medium-frequency bath. It is shown that the decoherence and relaxation times of the qubit in the SIB model increase with the decrease of the oscillation frequency $\Omega_0$ of the IHO, which is similar to the case that the bath has high frequencies.

**IV. CONCLUSIONS AND DISCUSSIONS**

In this paper we have investigated the decoherence and relaxation of a qubit coupled to an Ohmic bath directly and via an IHO. In our investigations, we fix the tunneling splitting $\Delta$ of the qubit. Two kinds of cases complementing paper I are discussed. The first is that the frequencies of the bath modes are low, and the IHO is far off the resonance to the bath modes, i.e. the oscillation frequency of the IHO is larger than the high-frequency cut-off of the bath modes. The second is that the frequencies of the bath modes are medium and in the case the IHO resonate with some mode of the bath. Here, we suppose that, in SIB model, the value of the damping coefficient $\Gamma$ of the bath to the IHO is intermediate as supposed in paper I, which make the bath has shorter memory time and it is suitable for our using the ITM based on the QUAPI. By using the ITM numerical scheme we calculated the evolutions of the reduced density matrix elements of qubit in the two models. Some new results are obtained. (1) When the frequencies of the bath modes are low ($0 < \omega \leq 0.1\Delta$) the qubit in the SB and SIB models has almost the same decoherence and relaxation times. Here, we set $\lambda\kappa = 1$ other than $\lambda\kappa = 1050$ in paper I. If the damping of the bath to the IHO or (and) the IHO to the qubit increase, namely $\lambda\kappa$ increase, the decoherence and relaxation times of the qubit in SIB model will decrease, and vice versa. (2) When the frequencies of the bath modes are medium ($0.1\Delta < \omega \leq 11\Delta$) and $\lambda\kappa = 1$, the qubit in the SIB model will have longer decoherence and relaxation times than it has in the SB model. As $\lambda\kappa$ increase to 1.125, the qubit in SIB model will have same decoherence and relaxation times to the qubit in SB model has, but the $\rho_{11}$ decays to a bigger equilibrium value. (3) The decoherence and relaxation times of the qubit in the SIB model increase with the decrease of the oscillation frequency $\Omega_0$ of the IHO. (4) As point out in paper I that the decoherence and relaxation times of the qubit in the SB and SIB models will increase with the decrease of the $\epsilon$ and $\Delta$, which has also not been plotted in the paper. The longer decoherence and relaxation times are necessary for not only the qubits for making the quantum computers but also the electrons for transferring energy in biological systems. In order to make the qubits or electrons in the SIB model with longer decoherence and relaxation times we may try to make the $\Omega_0$ and $\lambda\kappa$ smaller.

If the qubits in SB and SIB in full-frequency ($0 < \omega \leq 100\Delta$), or in low- and medium-frequency ($0 < \omega \leq 11\Delta$), or medium- and high-frequency ($11\Delta < \omega \leq 100\Delta$) baths, how about the dynamics of the qubits? This is an interesting problem. But, because the effective bath in the frequency spectra has so long memory times that the ITM algorithm in fact can not be applied for investigating the dynamics of the qubit in these cases. So, some new methods is expected for the goal. In paper I and this paper, we suppose that the qubit couple to the Ohmic bath, or the IHO couple to the Ohmic bath. If we
set the qubit or the IHO couple to other baths, for example, sub-Ohmic and super-Ohmic baths, the method used in the two papers is also valid, but in order to make the calculations convergence one should recalculate the memory times of the baths and choose the $k_{\text{max}}$ again, so that $k_{\text{max}} \Delta t \gtrsim \tau_m$.

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Fig. 3
