Comparison of analytical and numerical methods and the effect of bath coupling on the quantum decoherence

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Abstract

The dynamics of a qubit in a structured environment is investigated theoretically. One point of view of the model is the spin-boson model with a Lorentz shaped spectral density. An alternative view is a qubit coupled to harmonic oscillator (HO), which in turn coupled to a Ohmic environment. Two different methods are applied and compared for this problem. One is a perturbation method based on a unitary transformation. Since the transformed hamiltonian is of rotating wave approximation (RWA) form, we call it the transformed rotating wave approximation (TRWA) method. And the other one is the numerically exact method of the quasi-adiabatic propagator path-integral (QUAPI) method. TRWA method can be applied from the first point of view. And the QUAPI method can applied from both points of views. We find that from the 1st point of view QUAPI only works well for large Γ. Since the memory time is too long for the practical evaluation of QUAPI when Γ is small. We call this treatment as QUAPI1. And from the 2nd point of view, QUAPI works well for small Γ, since the non-adiabatic effect become more important as Γ increases, one need smaller time-step and more steps to obtain accurate result which also quickly runs out the computational resources. This treatment is called QUAPI2. We find that the TRWA method works well for the whole parameter range of Γ and show good agreement with QUAPI1 and QUAPI2. On the other hand, we find that the decoherence of the qubit can be reduced with increasing coupling between HO and bath. This result may be relevant to the design of quantum computer.

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I. INTRODUCTION

Dissipative quantum dynamics is of crucial interest among scientists. Since the quantum dynamics are always inevitably affected by its environment, various physical and chemical phenomena are related to the dissipation, range from the spontaneous emission to electron transfer in molecular, from qubit decoherence to photon harvest in photosynthesis \[1-5\]. Spin-boson model, the simplest possible model to describe dissipation, offers a comprehensive way to study the decoherence phenomenon. In the context of the electron transfer in molecular, spin boson model has been studied intensively over the past decades, and it shows revival interest among scientists because of the possible application of quantum computation and information.

For the spin boson model, the environmental property is characterized by the spectral density \(J(\omega)\), which is usually assumed to be a power law distribution, \(J(\omega) \propto \omega^s\), it is called sub-Ohmic when \(0 < s < 1\), Ohmic when \(s = 1\) and super-Ohmic when \(s > 1\). The most studied case is the Ohmic spectral density, it describes a case when the dissipation is the same at all frequencies, which is the case for the many environments. A physical example corresponds to the Ohmic case is the dissipation in a pure resistor circuit. For the sub-Ohmic case, it arouse lots of interest recently, because of the controversy related to the quantum phase transition. \[6-14\].

In this work, we study the dynamics of a qubit in a structured environment. Two points views are available for the problem we are interested in. One point of view is the spin boson model with a Lorentz shaped spectral density. And the alternative view is a two-level system (TLS) coupled to harmonic oscillator (HO), which in turn coupled to a Ohmic environment. The model describes some situations in experiments. For example, a flux qubit is usually read out by a dc-SQUID with a characteristic plasma frequency, consequently, the environmental noise of the SQUID is also transferred to the qubit leading to decoherence and dissipation. It also describes a Cooper-pare box (CPB) coupled to a transmission line resonator or a qubit placed in a leaky cavity.

From the first point of view, many tradition treatment of spin-boson model can be applied, some of them are largely numerical, such as the quantum Monte Carlo \[15-17\], real-time renormalization group \[18\], quasi-adiabatic path integrals (QUAPI) \[19-22\], flow equation renormalization (FER) \[23-28\] and numerical renormalization group (NRG) \[7\].
others are mainly analytical such as the non-interacting blip approximation (NIBA) \cite{27,31-34}, rigorous Born approximation \cite{25,35} or Bloch-Redfield \cite{36,37}, and the transformed rotating-wave approximation (TRWA) method \cite{38-41}. Till now, for this particular spectral density, it has been studied by FER \cite{26-28}, NIBA \cite{27,33}, Bloch-Redfield \cite{27} and TRWA \cite{40,41}. And from the second point of view, it has been studied by QUAPI \cite{22}, the van Vleck perturbation theory together with a Born-Markov master equation (VVBM) \cite{42}, Redfield equation based on a single mode TRWA \cite{43}. Although it has been studied intensively, the most studied case is the weak HO-bath coupling. While in this work, we explore the qubit decoherence in both the weak and strong HO-bath coupling regimes.

One commonly believed concept is that temperature and the coupling to noisy bath only play a negative role in preserving the qubit coherence. However, it is pointed out in Ref. \cite{44} that the temperature can help the coherence when the qubit is coupled to a TLF (or spin-boson) environment. We would like to ask: Is it possible to reduce the decoherence by increasing the system-bath coupling? In this paper, we examine the coupling effect on the quantum decoherence, we study aforementioned problem from the 1st point of view by the TRWA method in both the weak and strong HO-bath coupling regimes. To check the result, we also use the numerically exact method of the quasi-adiabatic propagator path-integral (QUAPI) method. We find that from the 1st point of view QUAPI only works well for large $\Gamma$. Since the memory time is too long for the practical evaluation of QUAPI when $\Gamma$ is small. We call this treatment as QUAPI1. And from the 2nd point of view, QUAPI works well for small $\Gamma$, since the non-adiabatic effect of the Ohmic bath become more important as $\Gamma$ increases, consequently, smaller time-step is required, thus, for the same memory time, one need more steps to obtain accurate result which also quickly runs out the computational resources. This treatment is called QUAPI2. We find that the TRWA method works well for the whole parameter range of $\Gamma$ and show good agreement with QUAPI1 and QUAPI2. On the other hand, we find that the decoherence of the qubit can be reduced with increasing HO-bath coupling when the HO-bath coupling is larger than the qubit-HO coupling.

The paper is organized as follows. In sec. II we present explicitly the two points of views of the problem we are interested in. In sec. III and IV we briefly introduce the TRWA and the QUAPI method, and discuss how to adopt these methods. In sec. V the coupling effect on the quantum coherence is discussed and a comparison of the TRWA with QUAPI is given. Finally, a brief conclusion is presented in Sec. VI.
II. TWO DIFFERENT POINTS OF VIEWS OF THE PROBLEM

The 1st point of view of the problem is the spin-boson model (un-biased case)

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

where $\sigma_x$ and $\sigma_z$ are the pauli matrices, $\Delta$ is the gap of the qubit, $b_k$ (or $b_k^\dagger$) are the annihilation (or creation) operators of the bath. And the spectral density is Lorentzian,

$$J(\omega) \equiv \sum_k g_k^2 \delta(\omega - \omega_k) = \frac{2\alpha \omega \Omega^4}{(\Omega^2 - \omega^2)^2 + (2\pi \Gamma \omega \Omega)^2}. \hspace{1cm} (2)$$

This spectral density possesses a shape peak at position $\Omega$ especially when $\Gamma$ is small, which may challenge the conventional method of the spin boson model. In the limit of $\Omega \to \infty$, $J(\omega)$ is reduced to the Ohmic spectral density.

The above model can be exactly mapped to a model where the qubit is dissipated by a multi-mode Ohmic bath via a harmonic oscillator, which is the 2nd point of view of this problem [45, 46]. The Hamiltonian reads ($\hbar = 1$)

$$H = \frac{\Delta}{2} \sigma_x + \Omega B^\dagger B + \sum_k \tilde{\omega}_k \tilde{b}_k^\dagger \tilde{b}_k$$
$$\quad \quad + (B^\dagger + B) \left[ g_0 \sigma_z + \sum_k \kappa_k (\tilde{b}_k + \tilde{b}_k^\dagger) \right] + (B^\dagger + B)^2 \sum_k \frac{\kappa_k^2}{\tilde{\omega}_k}, \hspace{1cm} (3)$$

where, $B$ (or $B^\dagger$) are the annihilation (or creation) operators of the HO, $\tilde{b}_k$ (or $\tilde{b}_k^\dagger$) are the annihilation (or creation) operators of the corresponding bath mode. The last term is the counter-term, which cancels the additional contribution due to the coupling of the HO to the bath [32, 47]. The corresponding spectral density is of Ohmic form

$$\tilde{J}(\omega) \equiv \sum_k \kappa_k^2 \delta(\omega - \tilde{\omega}_k) = \Gamma \omega e^{-\omega/\omega_c} \hspace{1cm} (4)$$

where $\omega_c$ is the cut-off frequency (throughout this work, we use the value $\omega_c = 20\Omega$). The relation between $g_0$ and $\alpha$ follows as $g_0 = \Omega \sqrt{\frac{\kappa}{8\Gamma}}$. From this 2nd point of view, the over all system TL plus HO can be considered as the system which is then dissipated by an Ohmic bath.

III. TRANSFORMED ROTATING-WAVE APPROXIMATION METHOD

The transformed rotating-wave approximation method is developed by one of the author and then applied to a sequence of problems [38, 41, 48–60]. Our starting point is the SBM...
with the structured spectral density. A unitary transformation is first applied to the SBM Hamiltonian, $H' = \exp(S)H \exp(-S)$, with the generator $S \equiv \sum_k \frac{g_k}{\omega_k} \xi_k (b_k^\dagger - b_k)\sigma_z$. The transformed Hamiltonian can be decomposed into three parts:

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

(5)

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

(6)

$$H'_2 = -\frac{\sigma_x}{2} \Delta \{ \cosh X - \eta \} - \frac{i\sigma_y}{2} \Delta \left\{ \sinh X - \eta X \right\},$$

(7)

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

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

(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 direct product: $|s\rangle \{|n_k\rangle\}$, where $|s\rangle$ is the eigenstate of $\sigma_x$ and $\{|n_k\rangle\}$ is the eigenstate of 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 spin and $\{|0_k\rangle\}$ stands for the vacuum state of the bosons.

The choice of $\eta$ in Eq. (8) insures $H'_2$ contains only the terms of two-boson and multiboson 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. If we let $H'_1|g_0\rangle = 0$, which ensures $H'_1$ to be small and more suitable for the subsequent perturbation treatment, then the parameters $\xi_k$’s are determined as,

$$\xi_k = \frac{\omega_k}{\omega_k + \eta \Delta}.$$

(9)

Consequently, $H'_1$ is transformed to the rotating-wave form,

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

where $V_k = \eta \Delta g_k \xi_k / \omega_k = g_k \eta \Delta / (\omega_k + \eta \Delta)$ and $\sigma_\pm \equiv (\sigma_z \mp i\sigma_y) / 2$. 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 $V_k$. Note that $\xi_k \sim 1$ if the boson frequency $\omega_k$ 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 of bosons, 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 $\omega_k \sim \eta \Delta$ 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 $\xi_k \ll 1$.

The total density matrix (system+environment) $\chi(t)$ obeys the Liouville-von-Neumann equation,

$$\frac{d}{dt} \tilde{\chi}(t) = -i[\hat{H}_1(t), \tilde{\chi}(t)],$$
(10)

where the tildes denote operators in the interaction picture with respect to $H'_0$. Iterating up to the second order and tracing out the environmental degrees, one get the master equation within the Born approximation,

$$\frac{d}{dt} \tilde{\rho}(t) = -i\text{Tr}_B[\hat{H}_1(t), \tilde{\rho}_B \otimes \tilde{\rho}(0)] - \int_0^t dt'\text{Tr}_B[\hat{H}_1(t'), [\hat{H}_1(t'), \tilde{\rho}_B \otimes \tilde{\rho}(t')]],$$
(11)

where $\tilde{\rho}$ is the reduced density matrix $\tilde{\rho}(t) = \text{Tr}_B[\chi(t)]$, and $\tilde{\chi}(t)$ is replaced by an approximate factorized density matrix $\tilde{\chi}(t) \approx \rho_B \otimes \tilde{\rho}(t)$. The environment is usually assumed to remain in thermal equilibrium $\rho_B = e^{-\beta H'_0}/\text{Tr}e^{-\beta H'_0}$ with $H'_B = \sum_k \omega_k b_k^\dagger b_k$, which is justified when the environment is 'very large' and the coupling 'weak' ($V_k \ll \Delta, \Omega$), so that the back-action of the system onto the environment can be neglected. Substitute $H'_1$ into the master equation, we get

$$\frac{\partial \tilde{\rho}(t)}{\partial t} = -i\text{Tr}_B[H'_1, \tilde{\rho}(t)] - \sum_k V_k^2 \int_0^t dt' \tilde{X}(t, t')$$
(12)

where,

$$\tilde{X}(t, t') \equiv n_k[\sigma_-(t)\sigma_+(t')\tilde{\rho}(t') - \sigma_+(t')\tilde{\rho}(t')\sigma_-(t)]e^{i\omega_k(t-t')}$$
$$+ n_k[\tilde{\rho}(t')\sigma_-(t')\sigma_+(t) - \sigma_+(t')\tilde{\rho}(t')\sigma_-(t)]e^{-i\omega_k(t-t')}$$
$$+ (n_k + 1)[\sigma_-(t)\sigma_-(t')\tilde{\rho}(t') - \sigma_-(t')\tilde{\rho}(t')\sigma_-(t)]e^{-i\omega_k(t-t')}$$
$$+ (n_k + 1)[\tilde{\rho}(t')\sigma_+(t')\sigma_-(t) - \sigma_-(t)\tilde{\rho}(t')\sigma_+(t')]e^{i\omega_k(t-t')}$$

The master equation Eq. (12) which is a $2 \times 2$ matrix equation can be solved exactly by the Laplace transform since the convolution theorem can be applied to the equation of each
matrix element. Here, for simplicity, we only present the comparatively brief expression. Suppose the system is in the upper eigenstate of $\sigma_z$ at time $t = 0$. At the zero temperature, the population difference $P(t) \equiv \langle \sigma_z(t) \rangle \equiv \text{Tr}_A(\sigma_z \rho(t))$ is evaluated as

$$P(t) = \frac{1}{\pi} \int_0^\infty d\omega \frac{\gamma(\omega) \cos(\omega t)}{[\omega - \eta \Delta - R(\omega)]^2 + \gamma^2(\omega)}. \quad (13)$$

$R(\omega)$ and $\gamma(\omega)$ in Eq. (13) are the real and imaginary parts of $\sum_k V_k^2/(\omega - \nu^+ - \omega_k)$

$$R(\omega) = \int_0^\infty d\omega' \frac{(\eta \Delta)^2 J(\omega')}{(\omega' + \eta \Delta)^2(\omega - \omega')}, \quad (14)$$

$$\gamma(\omega) = \pi J(\omega)(\eta \Delta)^2/(\omega + \eta \Delta)^2. \quad (15)$$

IV. QUASI-ADIABATIC PATH-INTEGRAL METHOD

The QUAPI method is a numerical scheme based on a exact methodology [19–22]. The starting point of QUAPI method is the generic system-bath Hamiltonian

$$H = H_0 + \sum_j \frac{P_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 (Q_j - c_j s/m_j \omega_j^2)^2.$$

where, $H_0$ is the Hamiltonian for the bare system, $s$ is the system coordinate, and $Q_j$ are harmonic bath coordinates which are linearly coupled to the system coordinate. The characteristics of the bath are captured in the spectral density function

$$J(\omega) = \frac{\pi}{2} \sum_j \frac{c_j^2}{m_j \omega_j} \delta(\omega - \omega_j). \quad (16)$$

The reduced density matrix of the system evolve as $\rho(s'', s', t) = \text{Tr}_{bath} \langle s''| e^{-iH_0 t} \rho(0) e^{iH_0 t} | s' \rangle$. If the path integral representation is discretized by $N$ time steps of length $\Delta t = t/N$ and the initial density matrix is assumed to be $\rho(0) = \rho_s(0) \rho_{bath}(0)$, the reduced density matrix takes the form

$$\rho(s'', s', t) = \sum_{s_{N-1}^+ s_{N-1}^-} \cdots \sum_{s_1^+ s_1^-} \sum_{s_0^+ s_0^-} \sum_{s''} \langle s''| e^{-iH_0 \Delta t} | s_{N-1}^+ \rangle \cdots \langle s_1^+ | e^{-iH_0 \Delta t} | s_0^+ \rangle$$

$$\langle s_0^+ | \rho_s(0) | s_0^- \rangle \langle s_0^- | e^{iH_0 \Delta t} | s_1^- \rangle \cdots \langle s_{N-1}^- | e^{iH_0 \Delta t} | s' \rangle \hat{I}(s_{N-1}^+, s_1^+, s_1^-, \cdots, s_{N-1}^+, s_{N-1}^-, s'', s', \Delta t)$$

$$\quad (17)$$

where the discrete variable representation (DVR) is used, the symbol $s_k^\pm (k = 0 \ldots N - 1)$ denotes the system coordinate at the time $k\Delta t$ on the forward and backward discretized
Feynman path. $|s_k^\pm\rangle$ ($k = 0, ..., N - 1$) are the eigenstates of the system coordinate operator $s$. If a symmetric splitting of the time-evolution operator is employed $e^{-iH\Delta t} = e^{-iH_{\text{env}}\Delta t/2}e^{-iH_0\Delta t}e^{iH_{\text{env}}\Delta t/2}$ with $H_{\text{env}} = H - H_0$, the corresponding influence functional reads

$$I(s_0^+, s_0^-, s_1^+, s_1^-, \ldots, s_{N-1}^+, s_{N-1}^-, s_N^+, s_N^-, \Delta t) = \text{Tr}_{\text{bath}} \left[ e^{-iH_{\text{env}}(s')\Delta t/2}e^{-iH_{\text{env}}(s_{N-1}^+)\Delta t} \ldots e^{-iH_{\text{env}}(s_0^+)\Delta t/2} \times \rho_{\text{bath}}(0)e^{iH_{\text{env}}(s_0^-)\Delta t/2} \ldots e^{iH_{\text{env}}(s_{N-1}^-)\Delta t}e^{iH_{\text{env}}(s')\Delta t/2} \right], \quad (18)$$

One can find that the equilibrium position of the bath mode is adiabatically displaced along the system coordinate. If $H_0$ provides a reasonable zeroth-order approximation to the dynamics, the quasi-adiabatic propagator is accurate for fairly large time steps. That is the quasi-adiabatic partitioning is a good representation when the bath property is mainly adiabatic, where the bath can keep up with the motion the system quickly. And the discrete path is to take into account of the non-adiabatic effect. For most of case, the quasi-adiabatic partitioning is reasonable especially when the system bath coupling is not strong. Therefore, the QUAPI discretization permits fairly large time steps when the adiabatic bath dominates the system dynamics. If the bath is purely adiabatic, even no discretization is needed. In the continuous limit (that is for $\Delta t \to 0, N \to \infty$) the influence functional has been calculated by Feynman and Vernon

$$I = \exp \left\{ -\frac{1}{\hbar} \int_0^t dt' \int_0^{t'} dt'' \left[ s^+(t') - s^-(t') \right] \times \left[ \alpha(t' - t'')s^+(t'') - \alpha^*(t' - t'')s^-(t'') \right] - i \frac{\hbar}{\Delta t} \sum_j \frac{c_j^2}{2m_j\omega_j^2} \left[ s^+(t')^2 - s^-(t')^2 \right] \right\} \quad (19)$$

where $\alpha(t)$ is the bath response function, which can be expressed in terms of the spectral density as

$$\alpha(t) = \frac{1}{\pi} \int_0^\infty d\omega J(\omega) \left[ \coth \left( \frac{\beta \omega_j \hbar}{2} \cos(\omega_j t) - i \sin(\omega_j t) \right) \right]. \quad (20)$$

The last term in Eq. (19) arises from the ”counter-terms” which are grouped with the bath Hamiltonian in the quasi-adiabatic splitting of the propagator. With the quasi-adiabatic discretization of the path integral, the influence functional, Eq. (19) takes the form

$$I = \exp \left\{ -\frac{1}{\hbar} \sum_{k=0}^{N} \sum_{k'=0}^{k} \left[ s_k^+ - s_k^- \right] \left[ \eta_{kk'} s_{k'}^+ - \eta_{kk'}^* s_{k'}^- \right] \right\}.$$
where $s_N^+ = s''$ and $s_N^- = s'$. The coefficients $\eta_{kk'}$ can be obtained by substituting the discretized path into the Feynman-Vernon expression Eq. (19), which is given in Ref. [20].

The QUAPI method is essentially a tensor multiplication scheme, which exploits the observation that for environments characterized by broad spectra the response function $\alpha(t)$ decays within a finite time interval. From the expression of the Feynman and Vernon influence functional Eq. (17), one can see that $\alpha(t)$ characterizes nonlocal interactions, which connects system coordinate $s(t')$ with $s(t'')$. The path $s^{\pm}(t')$ at time $t'$ is connected to all the paths $s^-(t'')$ at earlier times, which makes the evaluation of Eq. (17) a hard task. However, for a bath with a broad spectral density, such as a power law distribution of the spectral density, $\alpha(t)$ has the finite memory, the memory length typically extending over only a few time slices when the quasi-adiabatic propagator is used to discretize the path integral. After discarding the negligible "long-distance interaction" with $t' - t'' > \Delta k_{\text{max}} \Delta t$ (or $k - k' > \Delta k_{\text{max}}$), the resulting path integral can be evaluated iteratively by multiplication of a tensor of rank $2\Delta k_{\text{max}}$. In other words, there exists an augmented reduced density tensor of rank $\Delta k_{\text{max}}$ that obeys Markovian dynamics. The details of the multiplication scheme is discussed to a great extent in the literature, here we only present the essential parameters and mention briefly how to adopt it to our specific problem [19–22].

A. QUAPI1: treatment from the 1st point of view

The Quapi method is based on an exact methodology, and for most conventional bath, such as bath with power law distributed spectral density, QUAPI work efficiently and converge easily. However, for the spectral density studied here, it pose challenge to the application of the QUAPI method, since the memory length is too long for the practical implementation of the QUAPI when $\Gamma$ is small. The response function is depicted in Fig. 1, one can find that because of the characteristic peak frequency $\Omega$ of the spectral density, the response function possess a coherent oscillation with frequency $\Omega$, and possesses very long memory time. However, when $\Gamma$ becomes large, the damping of the kernel becomes significant, and the response function quickly damp to the zero. which en ables the application of the QUAPI. Here we discuss briefly the parameters used in the QUAPI1 method:

(i) The first parameter time-step $\Delta t$ used for the quasi-adiabatic splitting of the path-integral. The memory time of the non-Markovian steps used by QUAPI is $\Delta k_{\text{max}} \Delta t$. The
stability of the iterative density matrix propagation ensures the choices of $\Delta t$, it should not be too big nor too small, since the non-adiabatic effect requires more splitting of the path integral, that is smaller $\Delta t$. Whereas, since the memory length $\Delta k_{\text{max}} \Delta t$ is usually a fixed value for a particular bath, QUAPI method prefers larger $\Delta t$, and consequently smaller $\Delta k_{\text{max}}$ in consideration of the numerical efficiency (note that the algorithm scales exponentially with $\Delta k_{\text{max}}$, also see the discussion of the second parameter $\Delta k_{\text{max}}$). Therefore, we should choose appropriate $\Delta t$ to take into account both the non-adiabatic effect which prefer smaller time splitting and the non-Markov effect which prefer long memory time, typically, we choose $\Delta t$ around $\frac{2\pi}{20 \Delta}$, that is to choose tens of fraction of the cycle time of the bare system dynamics.

(ii) The second parameter is the memory steps $\Delta k_{\text{max}}$. If $\Delta k_{\text{max}} \leq 1$, the dynamics is purely Markovian. If the non-locality extends over longer time, terms with $\Delta k_{\text{max}} > 1$ have to be included to obtain accurate results. In order to acquire converge result, in the practical implementation of QUAPI, one usually need to choose $\Delta k_{\text{max}}$ large enough so that the response function reduces to negligible value within the length of $\Delta k_{\text{max}} \Delta t$. However this is a hard task, Since augmented propagator tensor $A^{(\Delta k_{\text{max}})}$ is a vector of dimension $(M^2)^{\Delta k_{\text{max}}}$ ($M$ is the system dimension which is two here), and the corresponding tensor propagator $T^{(2\Delta k_{\text{max}})}$ is a matrix of dimension $(M^2)^{2\Delta k_{\text{max}}}$, the QUAPI scheme scales exponentially with the parameter $\Delta k_{\text{max}}$. Thus one can not proceed the QUAPI calculation with very large $\Delta k_{\text{max}}$, and usually $\Delta k_{\text{max}}$ is chosen less than 10 for $M = 2$, and even smaller for larger $M$.

In summary, one have to select appropriate $\Delta t$ and $\Delta k_{\text{max}}$ to achieve stable and accurate result. As discussed in [20, 21] for the SBM problem with the ohmic bath, with the choice of $\Delta t = 0.25/\Omega$ ($\Omega$ is the tunneling rate of the bare system there), only $\Delta k_{\text{max}} = 5, 7$ reaches stability for zero bias (as shown in Fig. 2 in [20]) and only $\Delta k_{\text{max}} = 7, 9$ reaches the long time limit for nonzero bias (as shown in Fig. 5 in [20]). For our system, it is possible for the implementation of QUAPI only when $\Gamma$ is large enough, since the memory time is too long to implement QUAPI when $\Gamma$ is small.

**B. QUAPI2: treatment from the 2nd point of view**

As discussed above, the direct application of QUAPI method is impossible when $\Gamma$ is small, how ever, we can tackle this problem from the second point of view, that is qubit
is first coupled to a harmonic oscillator, which itself coupled to a Ohmic bath. Since the memory length of the Ohmic bath extend over only a few slices of the time steps. It enable the use of the QUAPI if we take the over all system of qubit-HO as the $H_0$ and the Ohmic bath as the environment. It work well especially for the weak $\Gamma$ in this case, since the nonadiabatic effect is weak for the small coupling and $H_0$ provides a reasonable zeroth-order approximation to the dynamics. Therefore $\Delta t$ can be fairly large, and the result converges quickly as $\Delta k_{\text{max}}$ increases.

However, since the qubit-HO system possess an infinite number of energy levels, it prohibit the direct use of the QUAPI. We have to truncate the qubit-HO system into a smaller sub-space for the practical implementation of the QUAPI method. Similarly to the Ref. [22], we first diagonalize the qubit-HO system in a large $N$ dimensional space and then only preserve the lowest $M$ energy eigenstates, consequently the system coordinate operator $X$ is also truncated to the $M$ dimension operator $X_M$ in the eigen energy representation. Then we diagonalize the $X_M$ to transform into the DVR basis. Since now the system is only $M$ dimensional, the implementation of QUAPI method becomes feasible.

Parameters in QUAPI2: (i) $\Delta t$ and (ii) $\Delta k_{\text{max}}$ are the same as QUAPI1. And two additional parameter appears in QUAPI2:

(iii) One parameter is the dimension $N$ of the Hilbert space of the qubit-HO system. The Hamiltonian of the qubit-HO system can be numerically diagonalized in the $N$ dimension of the Hilbert space. $N$ is kept fixed as $N = 400$ in our calculation, since it is big enough dimension for the diagonalization of the qubit-HO system.

(iv) Meanwhile, we have employed a second parameter $M$, which is the lowest energy sub-space of the dimension $N$ of the Hilbert space of the qubit-HO system. We first diagonalize the qubit-HO space in the larger dimension $N$ of the Hilbert space, to get more accurate low energy eigenstates and calculate the physical quantities in the $M$ dimension subspace with less numerical effort. Here we should choose larger $M$ for stronger qubit-HO coupling $g_0$.

V. RESULTS AND DISCUSSION

According to Eq. (2)-(8) and Eq. (13)-(15), $P(t)$ is obtained according to TRWA method. Here we report $P(t)$ as a function of time in Fig. 2 and Fig. 3 for the off-resonance case
For the off-resonance case as shown in Fig. 2 and Fig. 3, the decoherence is always enhanced by increasing the HO-boson coupling $\Gamma$ no matter that $\pi \Gamma \Delta$ is larger or smaller than $g_0$. However, for the on-resonance case, the decoherence is enhanced with increasing $\Gamma$ when $\pi \Gamma \Delta > g_0$ as shown in Fig. 4, whereas reduced with $\Gamma$ when $\pi \Gamma \Delta < g_0$ as shown in Fig. 5.

To check the peculiar results, we also calculate the population difference $P(t)$ by QUAPI method. For $\pi \Gamma \Delta > g_0$ we do the QUAPI from the first point of view (QUAPI1) and the result is reported in Fig. 3 and Fig. 5, the time splitting is set fixed as $\Delta t = 0.6/\Delta$ with varying memory steps $\Delta k_{\text{max}}$. In Fig. 5, one can find that when $\Gamma$ is large, i.e. $\Gamma = 0.4, 0.5$, it is easy for the calculation to converge and the result is good enough within $\Delta k_{\text{max}} = 3$. As $\Gamma$ decreases, it become harder for the evaluation because of the long memory time. In order to converge to our analytical result, it needs $\Delta k_{\text{max}} = 5$ for $\Gamma = 0.3$, $\Delta k_{\text{max}} = 7$ for $\Gamma = 0.2$, and even higher $\Delta k_{\text{max}}$ for $\Gamma = 0.1$ (which almost runs out our numerical resources). For even smaller $\Gamma$, such as $\Gamma = 0.02$, the evaluation from this point of view is practically impossible. Therefore, for $\pi \Gamma \Delta < g_0$ we do the QUAPI from the second point of view (QUAPI2), which is reported in Fig. 2 and Fig. 4. Here the time splitting is set fixed as $\Delta t = 0.15/\Delta$ in Fig. 2 and $\Delta t = 0.3/\Delta$ in Fig. 4, the dimension for diagonalization of TL-HO system is $N = 400$ and truncated dimension for QUAPI2 is $M = 2$ in Fig. 2 and $M = 6$ in Fig. 4. One can see that all these results converges to our TRWA results.

To understand the qubit behavior, we can explore the damping rate according to the TRWA method. One can find that in the near resonance case ($\Delta \approx \Omega$), level repulsion occurs, two characteristic frequencies dominate the qubit dynamics. When the HO-bath coupling is weak, the result should agree with that of the Jaynes-Cummings model, that is the peak frequency $\omega_p \approx \Delta \pm g_0$ [61]. Therefore, from Eq. (15), we get

$$\gamma_p \propto \frac{g_0^2 \Gamma}{g_0^2 + (\pi \Gamma \Delta)^2},$$

(21)

where we have approximated $\eta \approx 1, \omega_p + \eta \Delta \approx 2\Delta$ and $\omega_p + \Omega \approx 2\Delta$. Therefore, one expect $\gamma_p \propto \Gamma$ for $\pi \Gamma \Delta \ll g_0$ and $\gamma_p \propto \frac{1}{\Gamma}$ for $\pi \Gamma \Delta \gg g_0$, which is in accordance with the numerical results. Admittedly, as $\Gamma$ becomes larger, the above mentioned analysis is not a accurate, since the frequency shift of $\omega_p$ will become much more complex because of the dressing of phonons. However, from the numerical result, one can find the analysis captures the main physics of the coupling dependent behavior.
VI. CONCLUSION

In conclusion, the non-Markovian dynamics of a qubit under the decoherence of structured environment is investigated without RWA and Markov approximation. One point of view of the problem is the spin-boson model with a Lorentz shaped spectral density. An alternative view is a qubit coupled to harmonic oscillator (HO), which in turn coupled to a Ohmic environment. Two different methods are applied and compared for this problem. One is a TRWA method which is mainly analytical and the other one is the QUAPI method which is a numerical scheme based on an exact methodology. The TRWA method can be applied from the first point of view. And the QUAPI method can be applied from both points of views and called QUAPI1 and QUAPI2 respectively. QUAPI1 only works well for large $\Gamma$. Since the memory time is too long for the practical evaluation of QUAPI when $\Gamma$ is small. And QUAPI2 works well for small $\Gamma$, since the non-adiabatic effect become more important as $\Gamma$ increases, consequently smaller time-step $\Delta t$ and more memory steps $\Delta k_{max}$ are required to obtain accurate result which also quickly runs out the computational resources. We find that the TRWA method works well for the whole parameter range of $\Gamma$ and show good agreement with QUAPI1 and QUAPI2. On the other hand, we find that the decoherence of the qubit can be reduced with increasing coupling between HO and bath, which may be relevant to the design of quantum computer.

VII. ACKNOWLEDGEMENT

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[1] Y. Nakamura, Y. A. Pashkin, and J. S. Tsai, Nature 398, 786 (1999).
[2] I. Chiorescu, P. Bertet, K. Semba, Y. Nakamura, C. Harmans, and J. E. Mooij, Nature 431, 159 (2004), URL http://dx.doi.org/10.1038/nature02831
[3] J. Q. You and F. Nori, Phys. Today 58, 42 (2005).
[4] G. S. Engel, T. R. Calhoun, E. L. Read, T. K. Ahn, T. Mancal, Y. C. Cheng, R. E. Blankenship, and G. R. Fleming, Nature 446, 782 (2007), URL http://dx.doi.org/10.1038/nature05678
[5] H. Lee, Y. C. Cheng, and G. R. Fleming, Science 316, 1462 (2007), URL http://dx.doi.org/10.1126/science.1142188
[6] R. Bulla, N. H. Tong, and M. Vojta, Phys. Rev. Lett. 91 (2003), URL http://dx.doi.org/10.1103/PhysRevLett.91.170601
[7] F. B. Anders and A. Schiller, Phys. Rev. Lett. 95 (2005), URL http://dx.doi.org/10.1103/PhysRevLett.95.196801
[8] R. Bulla, H. J. Lee, N. H. Tong, and M. Vojta, Phys. Rev. B 71 (2005), URL http://dx.doi.org/10.1103/PhysRevB.71.045122
[9] M. Vojta, N. H. Tong, and R. Bulla, Phys. Rev. Lett. 94 (2005), URL http://dx.doi.org/10.1103/PhysRevLett.94.070604
[10] F. B. Anders, R. Bulla, and M. Vojta, Phys. Rev. Lett. 98 (2007), URL http://dx.doi.org/10.1103/PhysRevLett.98.210402
[11] F. B. Anders, New J. Phys. 10 (2008), URL http://dx.doi.org/10.1088/1367-2630/10/11/115007
[12] A. Winter, H. Rieger, M. Vojta, and R. Bulla, Phys. Rev. Lett. 102 (2009), URL http://dx.doi.org/10.1103/PhysRevLett.102.030601
[13] M. Vojta, N. H. Tong, and R. Bulla, Phys. Rev. Lett. 102 (2009), URL http://dx.doi.org/10.1103/PhysRevLett.102.249904
[14] M. Vojta, R. Bulla, F. Guttge, and F. Anders, Phys. Rev. B 81 (2010), URL http://dx.doi.org/10.1103/PhysRevB.81.075122
[15] R. Egger and U. Weiss, Zeitschrift f r Physik B Condensed Matter 89, 97 (1992), URL http://dx.doi.org/10.1007/BF01320834
[16] R. Egger and C. H. Mak, Phys. Rev. B 50, 15210 (1994), URL http://dx.doi.org/10.1103/PhysRevB.50.15210
[17] R. Egger, L. Mihlbacher, and C. H. Mak, Phys. Rev. E 61, 5961 (2000), URL http://dx.doi.org/10.1103/PhysRevE.61.5961
[18] M. Keil and H. Schoeller, Phys. Rev. B 63, 180302 (2001), URL http://dx.doi.org/10.1103/PhysRevB.63.180302
[19] D. E. Makarov and N. Makri, Chem. Phys. Lett. 221, 482 (1994), URL
[20] N. Makri and D. E. Makarov, J. Chem. Phys. 102, 4600 (1995), URL http://dx.doi.org/10.1063/1.469508

[21] N. Makri and D. E. Makarov, J. Chem. Phys. 102, 4611 (1995), URL http://dx.doi.org/10.1063/1.469509

[22] M. Thorwart, E. Paladino, and M. Grifoni, Chem. Phys. 296, 333 (2004), URL http://dx.doi.org/10.1016/j.chemphys.2003.10.007

[23] T. A. Costi and C. Kieffer, Phys. Rev. Lett. 76, 1683 (1996), URL http://dx.doi.org/10.1103/PhysRevLett.76.1683

[24] S. K. Kehrein and A. Mielke, Annalen Der Physik 6, 90 (1997).

[25] M. Grifoni, E. Paladino, and U. Weiss, Eur. Phys. J. B 10, 719 (1999).

[26] S. Kleff, S. Kehrein, and J. von Delft, Physica E 18, 343 (2003), URL http://dx.doi.org/10.1016/s1386-9477(02)01083-4

[27] F. K. Wilhelm, S. Kleff, and J. von Delft, Chem. Phys. 296, 345 (2004), URL http://dx.doi.org/10.1016/j.chemphys.2003.10.010

[28] S. Kleff, S. Kehrein, and J. von Delft, Phys. Rev. B 70, 014516 (2004), URL http://dx.doi.org/10.1103/PhysRevB.70.014516

[29] F. B. Anders and A. Schiller, Phys. Rev. B 74 (2006), URL http://dx.doi.org/10.1103/PhysRevB.74.245113

[30] R. Bulla, T. A. Costi, and T. Pruschke, Rev. Mod. Phys. 80, 395 (2008), URL http://dx.doi.org/10.1103/RevModPhys.80.395

[31] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. 59, 1 (1987), URL http://dx.doi.org/10.1103/RevModPhys.59.1

[32] U. Weiss, Quantum Dissipative Systems (World Scientific, Singapore, 1999), 2nd ed.

[33] F. Nesi, M. Grifoni, and E. Paladino, New J. Phys. 9, 316 (2007), URL http://dx.doi.org/10.1088/1367-2630/9/9/316

[34] F. Nesi, E. Paladino, M. Thorwart, and M. Grifoni, Phys. Rev. B 76 (2007), URL http://dx.doi.org/10.1103/PhysRevB.76.155323

[35] D. P. DiVincenzo and D. Loss, Phys. Rev. B 71 (2005), URL http://dx.doi.org/10.1103/PhysRevB.71.035318

[36] Redfield, Advan. Magnetic Reson. 1, 1 (1965).
[37] L. Hartmann, I. Goychuk, M. Grifoni, auml, and P. nggi, Phys. Rev. E 61, R4687 (2000), URL http://dx.doi.org/10.1103/PhysRevE.61.R4687

[38] H. Zheng, Eur. Phys. J. B 38, 559 (2004), URL http://dx.doi.org/10.1140/epjb/e2004-00152-7

[39] D. W. Wang, Z. H. Li, H. Zheng, and S. Y. Zhu, Phys. Rev. A 81 (2010), URL http://dx.doi.org/10.1103/PhysRevA.81.043819

[40] P. H. Huang and H. Zheng, J. Phys.: Condens. Matter 20, 395233 (2008), URL http://dx.doi.org/10.1088/0953-8984/20/39/395233

[41] C. J. Gan, P. H. Huang, and H. Zheng, J. Phys.: Condens. Matter 22, 115301 (2010), URL http://dx.doi.org/10.1088/0953-8984/22/11/115301

[42] J. Hausinger and M. Grifoni, New J. Phys. 10, 115015 (2008), URL http://dx.doi.org/10.1088/1367-2630/10/11/115015

[43] F. Brito and A. O. Caldeira, New J. Phys. 10, 115014 (2008), URL http://dx.doi.org/10.1088/1367-2630/10/11/115014

[44] A. Montina and F. T. Arecchi, Phys. Rev. Lett. 100, 120401 (2008), URL http://dx.doi.org/10.1103/PhysRevLett.100.120401

[45] A. Garg, J. N. Onuchic, and V. Ambegaokar, J. Chem. Phys. 83, 4491 (1985), URL http://dx.doi.org/10.1063/1.449017

[46] L. Tian, S. Lloyd, and T. P. Orlando, Phys. Rev. B 65, 144516 (2002), URL http://dx.doi.org/10.1103/PhysRevB.65.144516

[47] M. R. da Costa, A. O. Caldeira, S. M. Dutra, and H. Westfahl, Phys. Rev. A 61, 022107 (2000), URL http://dx.doi.org/10.1103/PhysRevA.61.022107

[48] Z. J. Wu, K. D. Zhu, X. Z. Yuan, Y. W. Jiang, and H. Zheng, Phys. Rev. B 71, 205323 (2005), URL http://dx.doi.org/10.1103/PhysRevB.71.205323

[49] K. D. Zhu, Z. J. Wu, X. Z. Yuan, and H. Zheng, Phys. Rev. B 71 (2005), URL http://dx.doi.org/10.1103/PhysRevB.71.235312

[50] X. F. Cao and H. Zheng, Phys. Rev. A 75 (2007), URL http://dx.doi.org/10.1103/PhysRevA.75.062121

[51] X. F. Cao and H. Zheng, Phys. Rev. B 76 (2007), URL http://dx.doi.org/10.1103/PhysRevB.76.115301

[52] Z. G. Lu and H. Zheng, Phys. Rev. B 75 (2007), URL
Figures Captions

Fig. 1: Real and imaginary parts of the bath response function for the Lorentzian spectral density. The memory time decreases to a finite range as $\Gamma$ increases.

Fig. 2: The population difference $P(t)$ as a function of time for the off-resonance case ($\Delta = 0.1\Omega$), the parameters are $g_0 = 0.1\Delta$ and $\pi\Gamma\Delta < g_0$, the QUAPI2 parameters are $N = 400$, $M = 2$, and $\Delta t = 0.15/\Delta$.

Fig. 3: The population difference $P(t)$ as a function of time for the off-resonance case ($\Delta = 0.1\Omega$), the parameters are $g_0 = 0.1\Delta$ and $\pi\Gamma\Delta > g_0$, the QUAPI1 parameter $\Delta t = 0.6/\Delta$.

Fig. 4: The population difference $P(t)$ as a function of time for the on-resonance case ($\Delta = \Omega$), the parameters are $g_0 = 0.1\Delta$ and $\pi\Gamma\Delta < g_0$, the QUAPI2 parameters are...
$N = 400$, $M = 6$, and $\Delta t = 0.3/\Delta$.

Fig. 5: The population difference $P(t)$ as a function of time for the on-resonance case $(\Delta = \Omega)$, the parameters are $g_0 = 0.1\Delta$ and $\pi \Gamma \Delta > g_0$, the parameters are $\Delta = \Omega$, $g_0 = 0.1\Delta$ and the QUAPI1 parameter $\Delta t = 0.6/\Delta$. 
FIG. 1: Fig. 1
FIG. 2: Fig. 2
FIG. 3: Fig. 3
FIG. 4: Fig. 4
FIG. 5: Fig. 5