Non-Markovian incoherent quantum dynamics of a two-state system

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We present a detailed study of the non-Markovian two-state system dynamics for the regime of incoherent quantum tunneling. Using perturbation theory in the system tunneling amplitude Δ, and in the limit of strong system-bath coupling, we determine the short-time evolution of the reduced density matrix and thereby find a general equation of motion for the non-Markovian evolution at longer times. We relate the nonlocality in time due to the non-Markovian effects with the environment characteristic response time. In addition, we study the incoherent evolution of a system with a double-well potential, where each well consists of several quantized energy levels. We determine the crossover temperature to a regime where many energy levels in the wells participate in the tunneling process, and observe that the required temperature can be much smaller than the one associated with the system plasma frequency. We also discuss experimental implications of our theoretical analysis.

I. INTRODUCTION

It is difficult to overemphasize the importance of the dissipative dynamics of a two-state system (TSS). In general, standing as a first hand approximation of a much rather complex level structure, the model of a TSS coupled to a dissipative environment[1,2] has been successfully applied to several physical systems. Indeed, the dissipative TSS dynamics is the paradigm for the study of superconducting devices containing Josephson junctions,[3] two-level atoms in optical cavities,[4] electron transfer in biological and chemical systems[5] and semiconductor quantum dots,[6] to name just a few.

Despite its simplicity, the description of the TSS dissipative dynamics imposes great theoretical challenges, especially when considering non-Markovian processes. This is the case for the analysis of the environment low-frequency noise spectrum, since the long-lived feature of its fluctuations does not allow for a "memoryless" bath (Markov) approximation. In the context of a weak TSS-bath coupling, theoretical efforts have been made to quantify the low-frequency effect for both spin-boson[7] and 1/f noise[8,9] models.

Furthermore, it has been largely demonstrated that low-frequency noise plays important role in the decoherence process of superconducting devices containing Josephson junctions.[10–14] Since those devices are seen as promising candidates to the physical implementation of a quantum bit, this subject has rapidly grown in interest and several studies on describing the microscopic origin and characterizing the low-frequency noise in such devices have already been put forward.[15–18]

Understanding the evolution of a TSS also plays an important role in understanding the performance of an adiabatic quantum computer[19] in the presence of noise.[20–23] This is because for many hard problems the bottleneck of the computation is passing through a point where the gap between the ground state and first-excited state is very small. Near such an energy anticrossing, the Hamiltonian of the system can be truncated into a two-state Hamiltonian[23] and in the

regime of strong coupling to the environment the two-state results discussed in this paper may be directly applied.

Here, following a previous work,[24] we put forward a detailed study of the TSS dissipative dynamics in the presence of low-frequency noise, for the regime of strong TSS-bath coupling. We show that, for the regime of small tunneling amplitude Δ, dephasing takes place much earlier in the evolution, leading the system to incoherent quantum dynamics. We employ such a property to derive equations that describe the non-Markovian evolution of the system's density matrix.

The paper is organized as follows. In Sec. II, we present the system Hamiltonian and a formal solution for the time evolution operator. Assuming second-order perturbation theory in Δ, we calculate in Sec. III the short-time dynamics of the system reduced density matrix elements. Section IV presents a discussion regarding the non-Markovian behavior of the system when the environment is in equilibrium. We determine conditions under which the system reaches the detailed balance regime. Section V provides a systematic derivation of an equation of motion for the system evolution, which in general is nonlocal in time. We also discuss regimes in which the equations governing the diagonal part of the density matrix become t-local. Considering a double-well potential, Sec. VI puts forward the analysis of intra- and interwell transitions and situations where a classical mixture of states participate in the quantum tunneling process. Finally, Sec. VII presents our concluding remarks.

II. SYSTEM HAMILTONIAN

We start by considering an open two-state system with Hamiltonian

$$H = -\frac{1}{2}[\Delta(t)\sigma_x + \epsilon(t)\sigma_z] - \frac{1}{2}\sigma_z Q + H_B, \qquad (1)$$

where Q is an operator acting on the environment described by the Hamiltonian H_B.

In order to determine the system evolution operator $U(t_2, t_1)$, we proceed through two simple steps. First, we

write the state vector of the system Hamiltonian (1) as $|\psi(t)\rangle = e^{iH_B t}|\varphi(t)\rangle$. ($\hbar = k_B = 1$ through this paper.) Thus, one finds that the state vector $|\varphi(t)\rangle$ evolves in time according to $i\frac{\partial}{\partial t}|\varphi(t)\rangle = [H_0(t) + V(t)]|\varphi(t)\rangle$, where

$$H_0(t) = -\frac{1}{2}\epsilon(t)\sigma_z - \frac{1}{2}\sigma_z Q(t), \quad V(t) = -\frac{1}{2}\Delta(t)\sigma_x, \quad (2)$$

and $Q(t) = e^{iH_B t}Q e^{-iH_B t}$. The environment is assumed to feature fluctuations following Gaussian distribution, therefore all averages can be expressed in terms of the correlation function or its Fourier transform, the spectral density:

$$S(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\langle Q(t)Q(0)\rangle, \quad (3)$$

hence we do not need to specify H_B.[25]

The next step is to make use of the interaction picture, considering $V(t)$ as the perturbation. The state vector in the interaction picture is defined by $|\varphi_I(t)\rangle \equiv U_0^\dagger(t)|\varphi(t)\rangle$, and any operator $\hat{O}$ is transformed by $\hat{O}_I(t) = U_0^\dagger(t)\hat{O}U_0(t)$, with

$$U_0(t) = \mathcal{T}e^{-i\int_0^t H_0(t')dt'} = \mathcal{T}\exp\left\{ i\frac{\sigma_z}{2}\int_0^t [\epsilon(t') + Q(t')]dt' \right\}, \quad (4)$$

where $\mathcal{T}$ denotes the time ordering operator. Now, the state evolution is determined by the interaction potential

$$H_I(t) = -\frac{1}{2}\Delta(t)\tilde{\sigma}_x(t), \quad (5)$$

where $\tilde{\sigma}_x(t) = U_0^\dagger(t)\sigma_x U_0(t)$. The time evolution operator in the interaction representation reads

$$U_I(t_2, t_1) = \mathcal{T}e^{-i\int_{t_1}^{t_2} H_I(t)dt}. \quad (6)$$

Finally, we can write a formal solution for the complete time evolution operator as

$$U(t_2, t_1) = \mathcal{T}e^{-i\int_{t_1}^{t_2} H(t)dt} = e^{-iH_B t_2}U_0(t_2)U_I(t_2, t_1)U_0^\dagger(t_1)e^{iH_B t_1}. \quad (7)$$

In this paper, we are interested in the strong coupling regime in which the root-mean-square value of the noise

$$W \equiv \sqrt{\langle Q^2 \rangle} = \left(\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S(\omega) \right)^{1/2}, \quad (8)$$

is much larger than the tunneling amplitude: $W \gg \Delta$. Physically, W is basically the uncertainty in the energy bias $\epsilon(t)$ and therefore represents the broadening of the energy levels. In the above regime, consequently, the broadening of the energy levels is larger than the minimum gap and therefore the gap will not be well defined. On the other hand, as we shall see, for the case of low-frequency noise, W represents the dephasing rate of the system. Thus, the above regime is a limit, in which the qubit loses quantum coherence before it can tunnel, i.e., the dynamics is incoherent.

III. DENSITY MATRIX CALCULATION

We would like to study the evolution of the reduced density matrix. Let $\rho_{SB}(t)$ denote the total density matrix of the system plus bath. We therefore have

$$\rho_{SB}(t) = U(t,0)\rho_{SB}(0)U^\dagger(t,0)$$
$$= e^{-iH_B t}U_0(t)U_I(t,0)\rho_{SB}(0)U_I^\dagger(t,0)U_0^\dagger(t)e^{iH_B t}. \quad (9)$$

The system reduced density matrix is defined by $\rho(t) = \text{Tr}_B[\rho_{SB}(t)]$, where $\text{Tr}_B[\dots]$ means averaging over all environmental modes. We assume that the density matrix at $t = 0$ is separable, i.e., $\rho_{SB}(0) = \rho(0) \otimes \rho_B$, where $\rho_B = e^{-H_B/T}$ is the density matrix of the environment, which we assume to be in equilibrium at temperature T. Under the assumption of separability of the initial density matrix, we consider that the system evolution immediately follows an initialization in a definite state, implemented, e.g., through a state measurement.

If Δ is the smallest energy scale in the problem, we can approximate $U_I(t,0)$ by performing a perturbation expansion in Δ, which up to second order reads

$$U_I(t,0) \approx 1 + \frac{i}{2}\int_0^t dt'\Delta(t')\tilde{\sigma}_x(t')$$
$$- \frac{1}{4}\int_0^t \int_0^{t'} dt'\,dt''\Delta(t')\Delta(t'')\tilde{\sigma}_x(t')\tilde{\sigma}_x(t''). \quad (10)$$

If the time interval t is not small enough to make the above integrals small, i.e., $t \gtrsim 1/\Delta$, the higher-order terms in Δ must be considered in the expansion.

A. Off-diagonal elements of ρ

To zeroth order in Δ, we have $U_I(t,0) = 1$, therefore

$$\rho_{SB}(t) = e^{-iH_B t}U_0(t)\rho_{SB}(0)U_0^\dagger(t)e^{iH_B t}. \quad (11)$$

For this case, since $[U_0(t), \sigma_z] = 0$, the σ_z populations of the system reduced density matrix ρ are constants of motion. Therefore, in the representation of the eigenstates of σ_z, $\sigma_z|0\rangle = -|0\rangle(\sigma_z|1\rangle = |1\rangle)$, only the off-diagonal elements of ρ present dynamics, which, due to the coupling to environment, decay in time. This case constitutes the one of a pure dephasing dynamics. It has been subject of interest for many areas, where several approaches have been used to calculate the off-diagonal elements of ρ. Few examples are the (a) spin-boson model assuming a power-law behavior for the spectral density of the bath;[27,28] (b) spin-fermion model,[29,30] and (c) spin-two-state fluctuators system.[8] Here, we consider a bosonic bath, but do not have to specify the form of the bath spectral density. To quantify this decay, let us write the reduced density matrix as

$$\rho(t) = \sum_{i,j=0,1} \rho_{ij}(t)|i\rangle\langle j|. \quad (12)$$

We find for the off-diagonal element

$$\rho_{01}(t) = \mathrm{Tr}_B[\langle 0|U_0(t)\rho_{SB}(0)U_0^\dagger(t)|1\rangle] = \rho_{01}(0)$$
$$\times \, e^{-i\int_0^t \epsilon(t')dt'} \left\langle \overset{\leftarrow}{\mathcal{T}} e^{-i/2\int_0^t Q(t')dt'} \mathcal{T} e^{-i/2\int_0^t Q(t')dt'} \right\rangle, \tag{13}$$

where $\langle \ldots \rangle \equiv \mathrm{Tr}_B[\rho_B \ldots]$ and $\overset{\leftarrow}{\mathcal{T}}$ represents the reverse time ordering operator. We expand the exponentials, group those in the same order, take the average of each term, and bring them back to the exponent. Because of the Gaussian nature of the environment, it is sufficient to expand up to second order in Q. One finds

$$\left\langle \overset{\leftarrow}{\mathcal{T}} e^{-i/2\int_0^t Q(t')dt'} \mathcal{T} e^{-i/2\int_0^t Q(t')dt'} \right\rangle = e^{-1/2\int_0^t dt' \int_0^t dt'' \langle Q(t')Q(t'')\rangle}$$
$$= e^{-1/2\int d\omega/2\pi \int_0^t dt' \int_0^t dt'' e^{i\omega(t''-t')}S(\omega)}. \tag{14}$$

Thus, using Eq. (14) in Eq. (13), we obtain

$$\rho_{01}(t) = e^{-i\int_0^t \epsilon(t')dt'} \times \exp\left\{-\int \frac{d\omega}{\pi} S(\omega) \frac{\sin^2(\omega t/2)}{\omega^2}\right\} \rho_{01}(0). \tag{15}$$

This equation represents a complicated decay rate, which is in general not a simple exponential function of t. However, in two limits it can be simplified. First, for the case of white noise, i.e., $S(\omega) = S(0)$, it gives

$$\rho_{01}(t) = e^{-i\int_0^t \epsilon(t')dt' - 1/2 S(0)t} \rho_{01}(0), \tag{16}$$

which leads to dephasing rate $1/t_\phi = \frac{1}{2}S(0)$, as expected for white noise.

Another interesting limit is when $S(\omega)$ is dominated by low frequencies so that one can use $\sin x \approx x$ to get

$$\rho_{01}(t) = e^{-i\int_0^t \epsilon(t')dt' - 1/2 W^2 t^2} \rho_{01}(0), \tag{17}$$

where W is the energy level broadening given by Eq. (8). The decay is now a Gaussian, whose width determines the dephasing rate, $1/T_\phi = W$. For the case of 1/f noise, where the cutoff of $S(\omega)$ is not sharp enough, one gets a logarithmic correction to the above equation.[8]

B. Diagonal elements of ρ

The evolution of the diagonal part of the density matrix happens in a time scale much larger than $1/W$. The complete evolution is given by

$$\rho(t) = \mathrm{Tr}_B[U_0(t)U_I(t,0)\rho(0)\rho_B U_I^\dagger(t,0)U_0^\dagger(t)]. \tag{18}$$

Let us assume the initial condition $\rho(0) = |0\rangle\langle 0|$ and try to calculate $\rho_{11}(t)$. To zeroth order in Δ, we have $\rho_{11}(t) = 0$ as expected, thus we find that the first nonzero contribution to $\rho_{11}(t)$ comes from the first-order term in Δ of (10):

$$\rho_{11}(t) \approx \frac{1}{4} \int_0^t dt_1 \int_0^t dt_2 \Delta(t_1)\Delta(t_2) \times \mathrm{Tr}_B[\langle 1|\tilde{\sigma}_x(t_1)|0\rangle \rho_B \langle 0|\tilde{\sigma}_x(t_2)|1\rangle]$$

$$= \frac{1}{4} \int_0^t dt_1 \int_0^t dt_2 \Delta(t_1)\Delta(t_2) \times \mathrm{Tr}_B[\langle 1|U_0^\dagger(t_1)U_0^*(t_1)|1\rangle \rho_B \langle 0|U_0^\dagger(t_2)U_0^*(t_2)|0\rangle]$$

$$= \frac{1}{4} \int_0^t dt_1 \int_0^t dt_2 \Delta(t_1)\Delta(t_2) e^{i\int_{t_1}^{t_2}\epsilon(t')dt'} \times \left\langle \overset{\leftarrow}{\mathcal{T}} e^{i/2\int_0^{t_2} Q(t')dt'} \mathcal{T} e^{i/2\int_0^{t_2} Q(t')dt'} \overset{\leftarrow}{\mathcal{T}} e^{-i/2\int_0^{t_1} Q(t')dt'} \mathcal{T} e^{-i/2\int_0^{t_1} Q(t')dt'} \right\rangle, \tag{19}$$

where in the second equality we have used $\tilde{\sigma}_x(t) = U_0^\dagger(t)\sigma_x U_0(t) = U_0^\dagger(t)U_0^*(t)\sigma_x$. One can calculate the expectation value by expanding the exponentials and keeping only the second order terms. The last two lines of Eq. (19) become

$$1 + \frac{1}{2}\int_0^{t_2} dt' \int_{t_2}^{t_1} dt'' \langle Q(t')Q(t'')\rangle$$
$$+ \frac{1}{2}\int_{t_1}^{t_2} dt' \int_0^{t_1} dt'' \langle Q(t')Q(t'')\rangle. \tag{20}$$

Substituting the inverse Fourier transformation $\langle Q(t')Q(t'')\rangle = \int \frac{d\omega}{2\pi} e^{-i\omega(t'-t'')}S(\omega)$, we find

$$1 + \int \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega^2} [e^{i\omega(t_1-t_2)} - 1 + i(\sin\omega t_2 - \sin\omega t_1)]$$

$$= 1 + \int \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega^2} (\cos\omega\tau - 1)$$

$$- i \int \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega^2} \left(\sin\omega\tau - 2\sin\frac{\omega\tau}{2}\cos\omega\tau'\right), \tag{21}$$

where $\tau = t_2 - t_1$ and $\tau' = (t_1 + t_2)/2$.

If the noise spectral density $S(\omega)$ is dominated by low-frequency noise such that for all relevant modes $\omega\tau \ll 1$, one can expand the $\sin\omega\tau$ and $\cos\omega\tau$ in Eq. (21) to get

$$\rho_{11}(t) \approx \frac{1}{4} \int_0^t d\tau' \int_{-\tilde{t}}^{\tilde{t}} d\tau \Delta\left(\tau' + \frac{\tau}{2}\right) \Delta\left(\tau' - \frac{\tau}{2}\right)$$

$$\times e^{-W^2\tau^2/2 - i(\epsilon_p(\tau')\tau - \int_{-\tau/2}^{\tau/2} \epsilon(\tau'+t')dt')}, \quad (22)$$

where $\tilde{t} = \min[2\tau', 2(t - \tau')]$, W is given by Eq. (8), and

$$\epsilon_p(t) \equiv \int \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega} (1 - \cos \omega t). \quad (23)$$

Equation (22) conveys the nonlocality in time, expected for a non-Markovian environment. If within time $\tau \sim 1/W$, $\epsilon(t)$ and $\Delta(t)$ do not change much (or even if $\Delta(t)$ is a fast but linear exponential function), we can write Eq. (22) as

$$\rho_{11}(t) \approx \frac{1}{4} \int_0^t d\tau' \Delta^2(\tau') \int_{-\tilde{t}}^{\tilde{t}} d\tau e^{i[\epsilon(\tau') - \epsilon_p(\tau')]\tau - W^2\tau^2/2}. \quad (24)$$

Therefore, for $t \lesssim 1/\Delta(t)$, we find the leading term for system population rate change given by

$$\dot{\rho}_{11}(t) \approx \frac{\Delta^2(t)}{4} \int_{-t}^t d\tau e^{i[\epsilon(t) - \epsilon_p(t)]\tau - W^2\tau^2/2}. \quad (25)$$

If $t > 1/W$, due to Gaussian envelope of the integrand, we can extend the integration limits of Eq. (25) to $\pm\infty$, obtaining

$$\dot{\rho}_{11}(t) \approx \Gamma_p e^{-[\epsilon(t) - \epsilon_p(t)]^2/2W^2}, \quad (26)$$

with the peak value of the functions given by

$$\Gamma_p \equiv \sqrt{\frac{\pi}{8}} \frac{\Delta^2}{W}. \quad (27)$$

It is worth recalling that for times $t \gtrsim 1/\Delta$, Eq. (10) does not represent a fair approximation to $U_I(t,0)$, hence the corrections to Eqs. (24)–(26), due to higher powers of Δ, become appreciable and must be considered.

In Sec V, we present a detailed study for the general equation of motion of the reduce density matrix consistent with Eq. (26). However, before we reach that stage, it is worth discussing a simpler system with a time independent Hamiltonian, and deriving some general features for $\epsilon_p(t)$ behavior.

IV. MACROSCOPIC RESONANT TUNNELING

Should ϵ_p be constant in time and the Hamiltonian (1) be time independent, one could directly read (26) as an approximation for the equation of motion

$$\dot{\rho}_{11}(t) \approx \Gamma_- \rho_{00}(t) - \Gamma_+ \rho_{11}(t), \quad (28)$$

since the off-diagonal elements of $\rho(t)$ become negligible for times $t \gtrsim 1/W$. The rate $\Gamma_-(\Gamma_+)$ then represents the $|0\rangle \rightarrow |1\rangle$ ($|1\rangle \rightarrow |0\rangle$) system transition rate. Thus, for the regime $1/W \lesssim t \lesssim 1/\Delta(t)$, the evolution is described by Eq. (26). The same argument holds when $\epsilon_p(t)$ is a function of time, but in that case the tunneling rates will be time dependent:

$$\Gamma_\pm(t) = \Gamma_p e^{-[\epsilon \pm \epsilon_p(t)]^2/2W^2}. \quad (29)$$

An experimental realization of such a tunneling process in a macroscopic quantum device such as a superconducting flux qubit is called macroscopic resonant tunneling (MRT). The tunneling rates $\Gamma_\pm$ are therefore simple shifted Gaussian functions described by Eq. (29). An immediate consequence of Eq. (23) is that the shift ϵ_p vanishes for a classical noise, for which $S(\omega)$ is symmetric. Therefore, a nonzero value of ϵ_p is a signature for quantum nature of the noise source.

If the environmental source is in equilibrium at temperature T, then the symmetric and antisymmetric (in frequency) parts of the noise intensity are related by the fluctuation-dissipation theorem:

$$S_s(\omega) = S_a(\omega) \coth\left(\frac{\omega}{2T}\right). \quad (30)$$

Therefore the fluctuation-dissipation theorem relates W and $\epsilon_p(t)$, which are functions of S_s and S_a, respectively. Let us first define

$$\epsilon_{p0} = \mathcal{P} \int \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega}, \quad (31)$$

with $\mathcal{P}$ representing principal value integral. In the case of low-frequency noise, when all the relevant frequencies are small on the scale of temperature T, i.e., $\omega \ll T$, one can write $\coth(\omega/2T) \simeq 2T/\omega$. In that case Eqs. (8), (30), and (31) yield

$$W^2 = 2T\epsilon_{p0}. \quad (32)$$

One therefore finds

$$\epsilon_p(t) = \epsilon_{p0} - \mathcal{P} \int \frac{d\omega}{2\pi} \frac{S(\omega)}{\omega} \cos \omega t. \quad (33)$$

The effect of the last term depends on how small or large t is with respect to the time response, $\tau_R \sim \omega_c^{-1}$, of the environment. Here, ω_c represents the characteristic energy of the environment. To understand this let us consider different regimes.

A. Large ω_c (short τ_R) limit

If ω_c is large compared to $1/t$, where t is the typical time scale of interest, then the integral in Eq. (33) covers many oscillations of the cosine function and therefore vanishes. In that case

$$\epsilon_p \approx \epsilon_{p0} = \frac{W^2}{2T}, \quad (34)$$

consequently being *independent* of t. For a time-independent Hamiltonian, Eq. (29) then yields

$$\Gamma_\pm(\epsilon) = \Gamma_p e^{-[\epsilon \pm \epsilon_{p0}]^2/2W^2}, \quad (35)$$

in agreement with Ref. 24. It is easy to see that

$$\frac{\Gamma_-(\epsilon)}{\Gamma_+(\epsilon)} = e^{\epsilon/T}, \quad (36)$$

which (in the limit $\Delta \rightarrow 0$) is the detailed balance (Einstein) relation. Therefore, the transition rates (35) support thermal equilibrium distribution of the system states, which is a natu-

ral consequence of the fast environmental response.

B. Small ω_c (long τ_R) limit

If the environment's response is slow compared to time scale of the problem, i.e., $\omega_c \ll 1/t$, the cosine function in Eq. (33) will be close to 1 at all times, making $\epsilon_p \approx 0$, again *independent* of t. For a time-independent Hamiltonian, therefore, we get

$$\Gamma_- = \Gamma_+ = \Gamma_p e^{-\epsilon^2/2W^2}. \tag{37}$$

Such transitions obviously do not satisfy the detailed balance relation and do not lead to equilibrium distribution.

Indeed, an environment in $\omega_c \to 0$ regime behaves as a static (classical) noise source. To see this, let us consider Hamiltonian (1) with a static noise source Q that does not vary much during the evolution and has a Gaussian distribution:

$$P(Q) = \frac{e^{-Q^2/2W^2}}{\sqrt{2\pi}W}. \tag{38}$$

In small Δ regime, the tunneling rate from state $|i\rangle$ to state $|j\rangle$ can be calculated using the Fermi Golden rule

$$\Gamma_{i \to j} = 2\pi |\langle i|V|j\rangle|^2 \delta(E_i - E_j), \tag{39}$$

where $V = \Delta\sigma_x/2$ is the perturbation potential. Therefore, for every realization of Q, one finds

$$\Gamma_-(Q) = \Gamma_+(Q) = \frac{\pi\Delta^2}{2}\delta(\epsilon + Q). \tag{40}$$

Averaging over all possibilities of Q, we find

$$\Gamma_- = \Gamma_+ = \frac{\pi\Delta^2}{2}\int dQ P(Q)\delta(\epsilon + Q) = \Gamma_p e^{-\epsilon^2/2W^2}, \tag{41}$$

which is the same as Eq. (37).

C. General ω_c (τ_R) regime

In general, away from the above two limits, $\epsilon_p(t)$ is a time-dependent function given by Eq. (33). The explicit functionality depends on the spectral density $S(\omega)$, especially on its characteristic frequency ω_c. To see this, let us assume a simple spectral density

$$S(\omega) = \frac{2\eta\omega}{[1 + (\omega/\omega_c)^2]^2}\left(\frac{1}{1 - e^{-\omega/T}}\right), \tag{42}$$

for which analytical solutions is possible. Substituting Eq. (42) in Eq. (33), we find

$$\epsilon_p(t) = \int \frac{d\omega}{2\pi}\frac{\eta(1 - \cos \omega t)}{[1 + (\omega/\omega_c)^2]^2} = \frac{\eta\omega_c}{4}[1 - e^{-\omega_c t}(1 + t\omega_c)], \tag{43}$$

We can therefore write

$$\epsilon_p(t) = \epsilon_{p0}(1 - e^{-\omega_c t}(1 + t\omega_c)) = \begin{cases} 0, & \omega_c t \ll 1 \\ \epsilon_{p0}, & \omega_c t \gg 1 \end{cases}, \tag{44}$$

which yields the above two limiting results in the appropriate regimes with an exponential crossover between the two lim-

its. Indeed, the above behavior of $\epsilon_p(t)$, i.e., the crossover from 0 to ϵ_{p0} within time scale $\sim 1/\omega_c$, is generic regardless of the functional detail of $\epsilon_p(t)$. The time scale $\tau_R \sim 1/\omega_c$ represents the response time of the environment to an external perturbation. If $t \gg \tau_R$, then the environment has enough time to enforce equilibrium to the system, resulting in $\epsilon_p = \epsilon_{p0}$, which is required for detailed balance (i.e., equilibrium) condition. On the other hand, if $t \ll \tau_R$, the environment cannot respond quickly to the system and the equilibrium relation is not expected. In that case, we find $\epsilon_p = 0$, i.e., the environment behaves as a classical noise. In the next section we shall see how such behavior results in time-nonlocality of the equation of motion.

V. NON-MARKOVIAN EQUATION OF MOTION

Equation (26) gives the short time ($1/W \lesssim t \lesssim 1/\Delta$) evolution of the diagonal part of the density matrix. As soon as t becomes comparable to Δ, higher order corrections become important and the second order perturbation used in Eq. (26) becomes insufficient. Instead of introducing higher-order corrections which is a cumbersome task, in this section we take a different path: We write a general equation of motion expected for the evolution of the density matrix for a system like ours and find its parameters in such a way that it agrees with Eq. (26) for short times.

In general, the equation of motion for the evolution of the density matrix is nonlocal in time, reflecting the non-Markovian nature of the environment. Since the off-diagonal elements vanish very quickly (within $t \sim 1/W$), for time scales larger than $1/W$, one can write the dynamical equations only in terms of the diagonal elements of ρ. Generally, for a non-Markovian dynamics the equation of motion for $\rho(t)$ depends on the history

$$\dot{\rho}_{11}(t) = \int_{-\infty}^{t} dt'[K_-(t,t')\rho_{00}(t') - K_+(t,t')\rho_{11}(t')], \tag{45}$$

where $K_\pm(t,t')$ are nonlocal integration kernels. Let us from now onwards consider a time-invariant Hamiltonian for which

$$\dot{\rho}_{11}(t) = \int_{-\infty}^{t} dt'[K_-(t-t')\rho_{00}(t') - K_+(t-t')\rho_{11}(t')]. \tag{46}$$

If the system starts the evolution from state $|0\rangle$ at time $t = t_0$, the short-time evolution is described by

$$\dot{\rho}_{11}(t) \approx \int_{t_0}^{t} dt' K_-(t-t') = \int_{0}^{t-t_0} d\tau K_-(\tau). \tag{47}$$

This should agree with Eq. (26), therefore

$$\int_{0}^{t-t_0} d\tau K_\pm(\tau) = \Lambda_\pm(t-t_0)\theta(t-t_0), \tag{48}$$

where we have defined functions

$$\Lambda_{\pm}(t) \equiv \Gamma_p e^{-[\epsilon \pm \epsilon_p(t)]^2/2W^2}. \qquad (49)$$

The presence of the θ-function is necessary to ensure causality to the system dynamics, since we assume that the evolution follows a state initialization at t_0. Taking the derivative of both sides of Eq. (48), we find

$$K_{\pm}(\tau) = \frac{\partial \Lambda_{\pm}(\tau)}{\partial \tau} \theta(\tau) + \Lambda_{\pm}(\tau)\delta(\tau). \qquad (50)$$

Notice that for constant transition rates $\Lambda_{\pm}(\tau) = \Gamma_{\pm}$, Eq. (50) leads to

$$\dot{\rho}_{11}(t) = \Gamma_- \rho_{00}(t) - \Gamma_+ \rho_{11}(t), \qquad (51)$$

which, as expected, is t-local.

In the limit $\omega_c \to 0$, where the change in $\Lambda_{\pm}$ happens on a time scale $(1/\omega_c)$ much larger than the time evolution considered here, the time derivative in Eq. (50) can be neglected and one obtains Eq. (51) with transition rates $\Gamma_{\pm} = \Lambda_{\pm}(0) = \Gamma_p e^{-\epsilon^2/2W^2}$, with $\epsilon_p(t) = 0$, as expected for a static noise.

On the other hand, in the $\omega_c \to \infty$ limit, variations of $\Lambda_{\pm}(t)$ happen in a very short time, hence $\partial \Lambda_{\pm}(\tau)/\partial \tau \to 0$ for $t \gtrsim \tau_R \sim 1/\omega_c$. Therefore the t' integration in Eq. (46) is basically between $t - \tau_R$ and t. If within this short range $\rho(t')$ does not change much, one can bring it outside the integral. In that case, Eq. (46) leads to Eq. (51) with $\Gamma_{\pm} = \Lambda_{\pm}(t \to \infty) = \Gamma_p e^{-(\epsilon \pm \epsilon_{p0})^2/2W^2}$, with $\epsilon_p(t) = \epsilon_{p0}$, which is expected in the detailed balance regime.

Both of the above regimes led to t-local equations for the diagonal part of the density matrix. However, for finite ω_c, in general, one gets a nonlocal equation in time. If the system evolution is slow compared to the time scale $\tau_R \sim 1/\omega_c$, one can substitute the Taylor expansion $\rho_{ij}(t') = \rho_{ij}(t) + (t' - t)\dot{\rho}_{ij}(t)$ into Eq. (46) obtaining

$$\dot{\rho}_{11}(t) = \Lambda_-(t)\rho_{00}(t) - \Lambda_+(t)\rho_{11}(t)$$
$$+ \dot{\rho}_{11}(t) \int_{t_0}^{t} dt' \frac{\partial \Lambda(t - t')}{\partial t}(t - t'), \qquad (52)$$

where $\Lambda(t) = \Lambda_-(t) + \Lambda_+(t)$. Solving for $\dot{\rho}_{11}(t)$, one finds Eq. (51) with transition rates

$$\Gamma_{\pm} = \frac{\Lambda_{\pm}(\infty)}{1 - \int_0^{\infty} d\tau\, \tau\, \partial \Lambda(\tau)/\partial \tau} = \frac{\Lambda_{\pm}(\infty)}{1 - \int_0^{\infty} d\tau [\Lambda(\infty) - \Lambda(\tau)]}, \qquad (53)$$

where in the last step we have used integration by parts. The integral limit was taken to infinity, since the integrand very quickly vanishes for $\tau \gtrsim 1/\omega_c$. All the nonlocal behavior is captured in the denominator of Eq. (53).

The integrand (53) is maximum at $\tau = 0$, but very quickly vanishes within $\tau \sim 1/\omega_c$, hence $\int_0^{\infty} d\tau [\Lambda(\infty) - \Lambda(\tau)] \sim [\Lambda(\infty) - \Lambda(0)]/\omega_c$, leading to

$$\Gamma_{\pm} \approx \frac{\Lambda_{\pm}(\infty)}{1 - [\Lambda(\infty) - \Lambda(0)]/\omega_c}. \qquad (54)$$

Using Eq. (49), we obtain

$$\Lambda(\infty) - \Lambda(0) = \Gamma_p(e^{-(\epsilon - \epsilon_{p0})^2/2W^2} + e^{-(\epsilon + \epsilon_{p0})^2/2W^2} - 2e^{-\epsilon^2/2W^2})$$
$$= 2\Gamma_p e^{-\epsilon^2/2W^2}\left(e^{-\epsilon_{p0}^2/2W^2}\cosh\frac{\epsilon}{2T} - 1\right). \qquad (55)$$

Therefore, to the lowest order in Γ_p/ω_c, we get

$$\Gamma_{\pm}(\epsilon) \approx \Gamma_p e^{-(\epsilon \pm \epsilon_{p0})^2/2W^2}$$
$$\times \left\{1 + \frac{2\Gamma_p}{\omega_c}e^{-\epsilon^2/2W^2}\left(e^{-\epsilon_{p0}^2/2W^2}\cosh\frac{\epsilon}{2T} - 1\right)\right\}. \qquad (56)$$

The magnitude and the position of the peak of $\Gamma_-(\epsilon)$ are given by (to the lowest order in Γ_p/ω_c)

$$\Gamma_{\text{peak}} \approx \Gamma_-(\epsilon_{p0}) \approx \Gamma_p(1 + \Gamma_p/\omega_c),$$

$$\epsilon_{\text{peak}} \approx \epsilon_{p0}\left(1 + \frac{2\Gamma_p}{\omega_c}e^{-\epsilon_{p0}^2/2W^2}\right). \qquad (57)$$

The peak value is enhanced by the nonlocal effects. The peak position is also shifted, but by a very small amount due to the exponential suppression. Notice that the peak becomes asymmetric around its center due to the nonlocality.

The nonlocal corrections to the transition rates become negligible when $\Gamma_p \ll \omega_c$. Also, observe that Γ_p is approximately the peak value of the transition rate (27). Therefore, nonlocality becomes important only when the maximum transition rate Γ_p is of the order of or larger than ω_c, or equivalently, when the response time (τ_R) of the environment is comparable or longer than the system transition time ($\sim 1/\Gamma_p$).

VI. MRT IN A DOUBLE-WELL POTENTIAL

So far we have studied incoherent tunneling in an idealized two-state system. However, for most realistic systems, the two-state model is only an approximation of a more complicated multilevel problem. An example of such cases is a system in which the classical potential energy has a double-well structure and the kinetic part of the Hamiltonian provides quantum tunneling between the two wells. Experimental implementation of such a system is possible using superconducting flux qubits, which have been studied considerably both theoretically and experimentally.[3,31–40] Especially, MRT measurements have been performed both between ground states as well as excited states of the wells.[37,38]

In such a double-well system, the energy within each well is quantized, with energy level distributions dependent on the bias energy between the wells. In general, in the presence of the environment, a system initialized in one of those levels can experience two types of evolution: intra- and interwell dynamics.

The intrawell dynamics are transitions within a single well, e.g., when a system excited within a well relaxes to a lower-energy level in the same well by exchanging energy with the environment. Thus, in this case, the system dynamics is confined in just one well of the potential, with no tunneling to the opposite well.

It is also possible for the system, depending on the tunneling amplitude between the two states, to tunnel to an en-

ergy level in the opposite well, leading thus to an interwell dynamics. If the evolution of the system is confined to the ground states of the two wells and it lies in the incoherent tunneling regime, then the formalism developed herein can describe such an evolution in full detail. This, however, is not the only type of evolution possible for a double-well system. Here, we also consider possibilities that the evolution involves the excited states.

A. Tunneling between ground states

At low enough temperatures, the system can only occupy the lowest energy states within the wells. In such a case, tunneling can occur between those energy levels if the levels become in resonance. The probability of the system being found in state $|1\rangle$ at time t is given by $\rho_{11}(t)$. For a time independent system initialized in state $|0\rangle$, in the limit $\Gamma_p \ll \omega_c$, $\rho_{11}(t)$ is the solution of Eq. (51). Such a t dependence can be measured experimentally and is usually an exponential function with initial value 0 and final value given by the equilibrium distribution. According to Eq. (51), the initial slope of $\rho_{11}(t)$ gives the transition rate: $\Gamma_- = \dot{\rho}_{11}(0)$. Likewise, if the system is initialized in state $|1\rangle$, one can extract Γ_+ in a similar way. Plotting the resulting transition rates versus bias ϵ, one obtains the tunneling resonant peaks. By fitting the experimental data to the shifted Gaussian lineshapes (35) the parameters ϵ_{p0}, W, and Γ_p can be extracted and from Eq. (27), Δ can be obtained. Such a procedure, performed in Ref. 38, successfully confirmed our theory especially the relation (32) between W and ϵ_{p0}.

If the transition rate Γ_p becomes comparable to the environment's characteristic energy ω_c, the t-local Eq. (51) will not be adequate to describe the evolution of the system. However, if the nonlocality effect is small, one can still use the same equation but with $\Gamma_\pm$ defined by Eq. (54), hence Eq. (56). In such a case, the peak will not be symmetric around its center, with an asymmetry that dependence on Δ. Experimental observation of such an asymmetry is an indication of time-delayed response of the environment and may provide information about ω_c. It should be reminded that a presence of high frequency modes in $S(\omega)$ may also lead to deviation from a symmetric Gaussian MRT peak but such an effect is independent of Δ hence could be easily distinguished from the above nonlocal effects.

Another interesting type of experiment is the Landau-Zener transition in which ϵ is a linear function of time during the evolution. For that type of evolution, again in the $\Gamma_p \ll \omega_c$ regime, one can still use (51) but with a time dependent ϵ. Such a procedure was proved successful in providing accurate description of the experimental data for flux qubits in Ref. 40.

It should be mentioned that the tunneling rate Δ in our formalism may not be independent of ϵ as assumed here. In practice, as the double-well potential is tilted, it not only affects the relative positions of the energy levels in the two wells but also affects the matrix elements between them. Such dependence is weak for a small bias, but as ϵ becomes large the effect of modulation of Δ might become visible.

B. Tunneling to or between excited states

If the energy tilt is large enough so that the ground state of the initial well becomes in resonance with an excited state of

the opposite well, tunneling to the excited state can occur. Alternatively, one may initialize the system in an excited state in the initial well, via, e.g., microwave excitation and make the system tunnel between two excited states. It is therefore important to understand how such a tunneling can be described within the present theory. One can generalize the arguments of the previous section to calculate the tunneling rate. In this case, we need to add intrawell relaxations to the picture.

In Ref. 24, it was shown that the tunneling rate from state $|i\rangle$ in the left well to state $|j\rangle$ in the right well is given by

$$\Gamma_{ij}(\epsilon) = \frac{\Delta_{ij}^2}{4} \int_{-\infty}^{\infty} dt\, e^{i(\epsilon - \epsilon_p)t - \gamma_{ij}|t| - 1/2 W^2 t^2}, \tag{58}$$

where ϵ is the bias energy with respect to the resonance point between $|i\rangle$ and $|j\rangle$, Δ_{ij} is the tunneling amplitude between the two states, and $\gamma_{ij} = (\gamma_i + \gamma_j)/2$, with γ_i being the intrawell relaxation rates corresponding to state $|i\rangle$. If one of the states is the ground state in its own well, then its corresponding intrawell relaxation rate is zero. The transition rate becomes a convolution of Lorentzian and Gaussian functions:

$$\begin{aligned}
\Gamma_{ij}(\epsilon) &= \frac{\Delta_{ij}^2 \gamma_{ij}}{\sqrt{8\pi} W} \int_{-\infty}^{\infty} d\epsilon' \frac{e^{-[\epsilon' - \epsilon_p]^2/2W^2}}{(\epsilon - \epsilon')^2 + \gamma_{ij}^2} \\
&= \sqrt{\frac{\pi}{8}} \frac{\Delta_{ij}^2}{W} \mathrm{Re}\left[w\left(\frac{\epsilon \pm \epsilon_p + i\gamma_{ij}}{\sqrt{2}W} \right) \right],
\end{aligned} \tag{59}$$

where

$$w(x) = e^{-x^2}[1 - \mathrm{erf}(-ix)] = \frac{2e^{-x^2}}{\sqrt{\pi}} \int_{ix}^{\infty} e^{-t^2} dt \tag{60}$$

is the complex error function. In the limit $\gamma_{ij} \to 0$, the shifted Gaussian lineshape (35) is recovered. In the opposite limit, $\gamma_{ij} \gg W$, the peak becomes a Lorentzian with width γ_{ij}.

C. Multichannel tunneling

So far, we have investigated the dynamics of a definite single tunneling event between the wells. However, as the system's temperature increases, one should expect the increase of probability of thermal occupation of the excited states of each well. Under such conditions, it becomes unknown what single tunneling event will take place. Consequently, when predicting the effective tunneling rate between wells, one has to take into account the statistics of occupation of excited states and their respective tunneling probabilities to the opposite well, in an ensemble average. The net of this thermally assisted dynamics is a multichannel tunneling, which leads to an increase of the measured tunneling rate. As we shall see, due to the fast increase of the tunneling amplitude Δ_{ij} between excited states $|i\rangle$ and $|j\rangle$, T does not need to be too large for this process to become non-negligible. For simplicity we consider zero bias ($\epsilon = 0$) situation in which the two potential wells are in resonance.

Let Δ_n and $\Gamma_\pm^n$ denote the tunneling amplitude and transition rate between the nth energy levels in the opposite wells, and $\Gamma_\pm$ the *total* transition rates between the wells. In ther-

mal equilibrium, the occupation probability of the nth state is given by Boltzmann distribution: $P_n = e^{-E_n/T}/\sum_i e^{-E_i/T}$. Therefore

$$\Gamma_\pm(\epsilon) = \sum_n P_n \Gamma_\pm^n(\epsilon). \tag{61}$$

At small enough T, one can assume $P_n \approx e^{-E_{n0}/T}$ (for $n > 0$), where $E_{n0} = E_n - E_0$ is the relative energy of state $|n\rangle$ compared to the ground state ($n = 0$). If $\gamma_{ij} \ll W$ for the low-lying energy levels, we may neglect γ_{ij} in Eq. (59) and all Γ_n will have the same Gaussian functional form, leading to

$$\Gamma_-(\epsilon) = \sum_n e^{-E_{n0}/T} \sqrt{\frac{\pi}{8}} \frac{\Delta_n^2}{W} e^{-[\epsilon-\epsilon_p]^2/2W^2},$$

$$= \sqrt{\frac{\pi}{8}} \frac{\Delta_{eff}^2(T)}{W} e^{-[\epsilon-\epsilon_p]^2/2W^2}, \tag{62}$$

where

$$\Delta_{eff} = \Delta_0 \left[1 + \sum_{n\geq 1} \frac{\Delta_n^2}{\Delta_0^2} e^{-E_{n0}/T} \right]^{1/2}. \tag{63}$$

Therefore, the net contribution from tunneling events involving excited states can be seen as a renormalization of the tunneling amplitude between wells. Since usually $\Delta_n \gg \Delta_0$, such contribution becomes important even at temperatures much smaller than the plasma frequency $\omega_p \equiv E_{10}$. The crossover temperature T_{co} can be obtained by requiring $(\Delta_1/\Delta_0)^2 e^{-\omega_p/T} \sim 1$, such that the contribution from the first excited state becomes important:

$$T_{co} = \frac{\omega_p}{2 \ln(\Delta_1/\Delta_0)}. \tag{64}$$

Typically Δ_1 is a few orders of magnitude larger than Δ_0 and therefore T_{co} can be an order of magnitude smaller than ω_p. High-frequency modes of environment may also renormalize the tunneling amplitude[1] resulting in a T-dependent Δ_{eff} even at $T < T_{co}$. Such a T dependence is typically much weaker and a crossover to the exponential dependence in Eq. (63) should be observable.

VII. CONCLUSIONS

We have shown a systematic procedure to determine the evolution of a two-state system in the regime of incoherent quantum dynamics. Considering a second-order perturbation theory in the system bare tunneling rate Δ, and a Gaussian distribution for the environment fluctuations, we have determined the short-time evolution of the system reduced density matrix elements.

Under the assumption of high integrated noise W, i.e., a system-bath strong coupling regime, we verify that, indeed, dephasing process takes place early in the system evolution, which sets $1/W$ as the smallest time scale of the evolution, justifying the claim of having a system with incoherent dynamics.

As for the system populations, we have seen that, in general, one should expect complex non-Markovian dynamics. We were able to clearly demonstrate how the non-Markovian evolution can be related to the time response of the environment, τ_R. Indeed, we have verified that for time scales $t \gg \tau_R$, the system follows the detailed balance dynamics. On the other hand, if the environment response is very slow, i.e., $t \ll \tau_R$, the system sees a static (classical) noise source. In addition, by investigating the equation of motion for the reduced density matrix, we have demonstrated how one can simplify the non-Markovian effects by introducing modified transition rates for the dynamical equations.

Finally, we have inspected the intra- and interwell transition possibilities inside a double-well potential, and quantified how the multichannel process can lead to an enhancement of the system tunneling. We have determined the condition for this process to take place, and estimated the crossover temperature which can be an order of magnitude smaller than the system plasma frequency ω_p.

Some of the predictions of our theory have already been confirmed experimentally.[38,40] More experiments, however, are necessary especially to confirm our description of non-Markovian dynamics. A simple measure of the asymmetry of the MRT peak in large Δ regime could be indicative of non-locality in t. As described in Sec. V, such an asymmetry should be Δ dependent and should disappear at small Δ. A Δ-independent asymmetry could result from high-frequency components of the environmental noise that make small $\omega\tau$ expansion in Eq. (21) fail. Moreover, a T-dependent measure of the tunneling rates can reveal the renormalization of the effective tunneling amplitude Δ due to high-frequency noise and the crossover temperature T_{co} to the multichannel tunneling regime as described in Sec. VI.

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