

Dissipative Landau-Zener transitions of a qubit: Bath-specific and universal behavior

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We study Landau-Zener transitions in a qubit coupled to a bath at zero temperature. A general formula that is applicable to models with a nondegenerate ground state is derived. We calculate exact transition probabilities for a qubit coupled to either a bosonic or a spin bath. The nature of the baths and the qubit-bath coupling is reflected in the transition probabilities. For diagonal coupling, when the bath causes energy fluctuations of the diabatic qubit states but no transitions between them, the transition probability coincides with the standard Landau-Zener probability of an isolated qubit. This result is universal as it does not depend on the specific type of bath. For pure off-diagonal coupling, by contrast, the tunneling probability is sensitive to the coupling strength. We discuss the relevance of our results for experiments on molecular nanomagnets, in circuit QED, and for the fast-pulse readout of superconducting phase qubits.

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I. INTRODUCTION

Nonadiabatic transitions at avoided level crossings play an essential role in numerous dynamical phenomena in physics and chemistry. They have been studied both theoretically and experimentally in various contexts such as spin-flip processes in nanoscale magnets,¹⁻⁴ molecular collisions,⁵ optical systems,^{6,7} quantum-dot arrays,⁸ Bose-Einstein condensates,⁹ the control of chemical reactions,¹⁰ and recently, in particular, in quantum information processing.¹¹⁻²⁰

The “standard” Landau-Zener (LZ) problem describes the ideal situation in which the dynamics is restricted to two levels that are coupled by a constant tunnel matrix element and cross at a constant velocity. The quantity of primary interest is the probability that finally the system ends up in one or the other of the two states. This classic problem was solved independently by several authors in 1932.²¹⁻²⁴ In quantum devices, not only the transition probability but also the nonadiabatic relative phase (Stokes phase) between the two states is important.^{8,12,15} This phase leads to observable interference effects, for example, in superconducting qubits.^{17,20}

In an experiment, the two-level system will be influenced by its environment, which may affect the quantum phase of the superposition, alter the effective interaction between the levels, or may cause spontaneous decay. For qubits in a solid-state environment,²⁵⁻²⁹ all these processes may occur simultaneously and hinder qubit manipulation. Thus, in the context of solid-state quantum information processing, a realistic study of qubit manipulation via Landau-Zener transitions should include the influence of environmental degrees of freedom.

The environment of a quantum system can often be described as a bath of harmonic oscillators.³⁰⁻³⁴ In some situations, it is known that the dominant environmental effects can be best modeled as a spin bath instead,³⁵⁻³⁷ for example, for molecular magnets^{3,4} and for Josephson phase qubits²⁷⁻²⁹ at very low temperatures.

In the presence of a heat bath, the Landau-Zener dynamics will sensitively depend on the qubit operator to which the bath couples.³⁸ Ao and Rammer^{39,40} studied the LZ problem for the special case in which an Ohmic heat bath couples to the same operator as the driving and derived the transition probabilities in the limit of high and of low temperatures. In the limits of very fast and very slow sweeps at zero temperature, they found that the transition probability is the same as in the absence of the heat bath, as was confirmed by numerical studies.^{41,42}

This zero-temperature result was recently proven to hold exactly for *arbitrary* Landau-Zener sweep speeds, as a special case of an exact expression for arbitrary qubit-bath couplings and spectral densities.³⁸ Very recently, Pokrovsky and Sun⁴³ developed an interesting finite-temperature formalism valid for baths with short correlation times, in which the exact transition probabilities of Ref. 38 indeed show up in the zero-temperature limit. At sufficiently high temperatures, the qubit experiences essentially classical Gaussian white noise and the Landau-Zener problem can be solved exactly.^{44,45}

A qubit that undergoes a Landau-Zener sweep while coupled to another quantum system is equivalent to a multilevel Landau-Zener problem in which two groups of levels cross. If all avoided crossings are sufficiently well separated, the dynamics consists of effectively independent transitions and one can compute the transition probabilities by transfer-matrix techniques.^{8,15,46,47} Independent level crossings do not occur for the dissipative Landau-Zener problem, for which the adiabatic energy spectrum is continuous. Other methods are therefore required, for example, the exact summation of a perturbation series.⁴⁴

Brundobler and Elser⁴⁸ considered a special multilevel Landau-Zener problem in which the system starts out in the diabatic state whose energy changes faster than that of all other diabatic levels. They conjectured that the transition probabilities are then given by an expression that only contains the velocities of the diabatic levels and off-diagonal matrix elements of the Hamiltonian. The conjecture has long

been known to be true for the exactly solvable Demkov-Osherov model, where *one* level crosses several parallel levels.^{48,49} Analytical proofs of the Brundobler-Elser conjecture have been given recently for several multilevel crossing situations.^{50–54}

The physically important situation of a two-level system coupled to a heat bath corresponds to two continuous bands of diabatic levels, with the same energy-level velocities within each band. A generalization of the theorem by Brundobler and Elser to this case will be considered. This general formula applies to dissipative Landau-Zener problems for all those kinds of baths at zero temperature for which the initial qubit-plus-bath ground state is unique. We discuss the implications of our results for a wide range of experiments for which these conditions are met. As one of our main results, we present a universal aspect of dissipative Landau-Zener transitions, independent of the precise nature of the bath.

The paper is organized as follows. In Sec. II we review the standard LZ formula for a two-level system and generalize it to the multilevel case; the explicit calculations have been deferred to the Appendix. Section III is devoted to the derivation of the LZ transition probability for both a harmonic-oscillator bath and a spin bath. In Sec. IV, we identify a universality in Landau-Zener tunneling that holds true even for baths of nonlinear oscillators. Finally, we discuss several promising applications and experiments in Sec. V.

II. LANDAU-ZENER TUNNELING PROBABILITIES

A. Landau-Zener transitions in an isolated qubit

To set the stage and to introduce our notation, we first review the standard Landau-Zener problem for an isolated qubit. By “isolated” we mean not coupled to an environment but nevertheless driven by a deterministic classical field, whose physical origin will be specified and discussed in Sec. V. The two-level Hamiltonian reads

$$\mathcal{H}_{\text{LZ}}(t) = \frac{vt}{2} \sigma_z + \frac{\Delta}{2} \sigma_x, \quad (1)$$

where $\sigma_z = |\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|$ and $\sigma_x = |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|$ are Pauli matrices while $|\uparrow\rangle$ and $|\downarrow\rangle$ denote the so-called diabatic states with the energies $\pm\frac{1}{2}vt$ which cross at $t=0$. Two parameters determine the dynamics: the constant sweep velocity $v > 0$, by which the energies of the diabatic states cross, and the coupling matrix element Δ between these states. Without loss of generality, we assume Δ to be real and non-negative. For $\Delta \neq 0$, the diabatic states are not eigenstates of the Hamiltonian (1), so that generally, a population transfer is induced. The Hamiltonian (1) is time dependent and so are its (adiabatic) eigenstates. In the limit $|t| \gg \Delta/v$, the adiabatic eigenstates coincide with the diabatic states.

The diabatic energies cross, but the adiabatic energies $\pm\frac{1}{2}\sqrt{v^2t^2 + \Delta^2}$ for $\Delta \neq 0$ form an avoided crossing, as sketched in Fig. 1. The adiabatic theorem⁵⁵ states that the splitting Δ prevents transfer of population between the adiabatic eigenstates in the adiabatic limit $\hbar v \ll \Delta^2$, in other words, if the sweep occurs slowly enough. A qubit prepared at $t = -\infty$ in the initial ground state $|\uparrow\rangle$ will then end up in the final

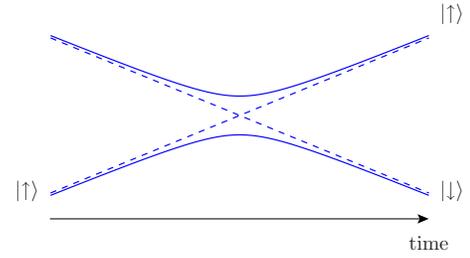


FIG. 1. (Color online) Adiabatic (solid) and diabatic (dashed) energies for the standard Landau-Zener problem.

ground state $|\downarrow\rangle$. Beyond the adiabatic regime, the dynamics can be rather complex. Nevertheless, the population of the diabatic states at $t = \infty$ can be calculated exactly and is determined by the Landau-Zener transition probability^{21–23}

$$P_{\uparrow \rightarrow \downarrow} \equiv |\langle \psi(\infty) | \downarrow \rangle|^2 = 1 - \exp\left(-\frac{\pi \Delta^2}{2 \hbar v}\right), \quad (2)$$

which denotes the probability for a *transition* to the opposite diabatic state, i.e., the probability to *stay* in the adiabatic eigenstate. Accordingly, $P_{\uparrow \rightarrow \uparrow} = 1 - P_{\uparrow \rightarrow \downarrow}$ denotes the probability for a nonadiabatic transition, i.e., a jump across the avoided crossing.

B. Landau-Zener transitions in nonisolated qubits

We now turn to situations where the qubit is no longer isolated. The Hamiltonian of the driven qubit plus its environment has the general form

$$\mathcal{H}(t) = \mathcal{H}_{\text{LZ}}(t) + \mathcal{H}_{\text{q-env}} + \mathcal{H}_{\text{env}}, \quad (3)$$

where \mathcal{H}_{env} describes the environment Hamiltonian with Hilbert space of dimension $M \leq \infty$. We assume the most general linear coupling between the qubit operators σ_x , $\sigma_y = -i(|\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow|)$, and σ_z and the environment operators $\mathcal{X}^{x,y,z}$; in other words, we take the qubit-environment coupling

$$\mathcal{H}_{\text{q-env}} = \sum_{\nu=x,y,z} \sigma_\nu \mathcal{X}^\nu. \quad (4)$$

We denote by $|k\rangle$ the eigenstates of the environment Hamiltonian \mathcal{H}_{env} .

An important assumption underlying our model Hamiltonian (3) is that the qubit-bath coupling (4) and the bath itself are not affected by the driving. Then, at very large times $t \rightarrow \pm\infty$, the qubit Hamiltonian is dominated by the time-dependent part, so that all states of the system-plus-environment belong to one of two bands: an “up cluster” $|\uparrow\rangle|k\rangle$ and a down cluster $|\downarrow\rangle|k\rangle$, with energies moving upward and downward, respectively.

1. Diabatic basis

The dissipative Landau-Zener problem is a scattering problem in the restricted sense that changes in the qubit’s state will occur only during a finite time interval around $t = 0$. In order to exploit this fact that the qubit will not flip for

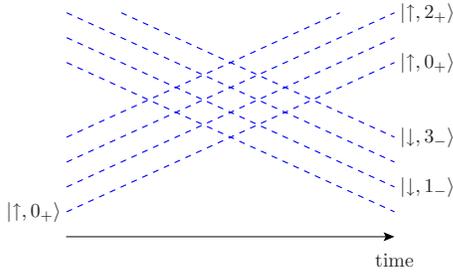


FIG. 2. (Color online) Sketch of the diabatic energy levels as a function of time for a qubit coupled to a *single* harmonic oscillator. Energies of the states in the up cluster increase. These states correspond to the qubit state $|\uparrow\rangle$. Energies decrease in the down cluster, where the qubit state is $|\downarrow\rangle$. According to the no-go-up theorem (A11), the initial state $|\uparrow, 0_+\rangle$ evolves to a superposition in which $|\uparrow, 0_+\rangle$ is the only “up” state. Energies within a band are separated by the oscillator energy $\hbar\Omega$. For a qubit coupled to an oscillator bath, the corresponding crossing clusters would be continuous bands of states.

sufficiently large $|t|$, we decompose $\mathcal{H}(t)$ into its diabatic states. These are the eigenstates of the total Hamiltonian (3) in the limits $t \rightarrow \pm\infty$. Initially and finally, the Hamiltonian is dominated by the term proportional to σ_z , so that the diabatic basis for the qubit is simply given by the states $|\uparrow\rangle$ and $|\downarrow\rangle$.

For the environment, by contrast, there is no corresponding growing energy scale for large $|t|$. Its diabatic states are influenced by the coupling to the qubit and depend on the qubit’s state. For the up cluster, these diabatic eigenstates of the environment are those which diagonalize the Hamiltonian projected to the subspace $|\uparrow\rangle$, i.e., $\langle\uparrow|\mathcal{H}|\uparrow\rangle$. They are eigenstates of $\mathcal{H}_{\text{env}} + \mathcal{X}^x$, and we denote them by $|k_+\rangle$ and their energies by ε_{k_+} . The diabatic bath states for the down cluster, $|k_-\rangle$, are defined likewise so that

$$(\mathcal{H}_{\text{env}} \pm \mathcal{X}^x)|k_{\pm}\rangle = \varepsilon_{k_{\pm}}|k_{\pm}\rangle. \quad (5)$$

The diabatic states of the qubit plus the bath read

$$|\uparrow k_+\rangle \equiv |\uparrow\rangle|k_+\rangle, \quad (6a)$$

$$|\downarrow k_-\rangle \equiv |\downarrow\rangle|k_-\rangle, \quad (6b)$$

where the labels $k_{\pm}=0,1,2,\dots$, are assigned such that the energies $\varepsilon_{k_{\pm}}$ are in increasing order, see the sketch in Fig. 2. At asymptotically large times, $t \rightarrow \pm\infty$, the diabatic states diagonalize the total Hamiltonian (3) and hence coincide with adiabatic eigenstates which diagonalize $\mathcal{H}(t)$ at a given time t . Note that $\langle\downarrow k_-|\uparrow k_+\rangle=0$, although in general $\langle k_+|k'_-\rangle \neq \delta_{kk'}$. A state of particular interest is the adiabatic ground state $|\uparrow 0_+\rangle$ which has energy $(vt/2 + \varepsilon_{0_+})$. At zero temperature, it is the natural initial state for the Landau-Zener dynamics.

We now split the Hamiltonian (3) into two parts, one that is diagonal in the spin index while the other is off-diagonal. The former part consists of all terms proportional to σ_z and is diagonal in the diabatic basis (6). The latter part reads

$$\mathcal{V} = \frac{\Delta}{2} \sigma_x + \sigma_x \mathcal{X}^x + \sigma_y \mathcal{X}^y \quad (7)$$

and will be called the *bit-flip interaction*, since it contains all interaction terms of the Hamiltonian (3) that induce a population change in the state of the qubit.

An important feature of the diabatic basis [Eq. (6)] is that all matrix elements of \mathcal{V} vanish within each cluster, i.e.,

$$\langle\uparrow k_+|\mathcal{V}|\uparrow k'_+\rangle = \langle\downarrow k_-|\mathcal{V}|\downarrow k'_-\rangle = 0. \quad (8)$$

This relation will be essential for the application of the general formula for the nonadiabatic transition probabilities as derived in the Appendix.

2. Nonadiabatic transition probabilities

We have now achieved a useful formulation of the dissipative Landau-Zener problem in terms of two groups of diabatic states. If the group of upward moving parallel levels would consist of merely one state, then transition probabilities could be computed with the simple independent-crossing formula, for which Brundobler and Elser⁴⁸ conjectured that it holds even when successive level crossings are not independent. Recent proofs show that the independent-crossing formula indeed holds exactly, even in more general situations.^{50–54} As stated above, for dissipative Landau-Zener transitions, there are two continua of states that cross with constant velocity. This physically important situation is addressed in the Appendix, where exact nonadiabatic transition probabilities are derived in a fairly general setting, with the crossing of two continua of parallel states as a special case. This setting is a generalization of our recent studies in Refs. 18 and 38.

For the dissipative Landau-Zener problem, we can deduce the following from Eqs. (A11) and (A21): If at $t=-\infty$ the system starts in a state $|\uparrow k_+\rangle$ whose diabatic energy is nondegenerate, then the following transition probabilities at $t=\infty$ are exact:

$$P_{\uparrow k_+ \rightarrow \uparrow k'_+} = \begin{cases} \exp\left(-\frac{2\pi\langle\uparrow k_+|\mathcal{V}^2|\uparrow k_+\rangle}{\hbar v}\right) & \text{for } k'_+ = k_+ \\ 0 & \text{for } k'_+ > k_+. \end{cases} \quad (9)$$

For the transition to lower states within the initial band of states ($k'_+ < k_+$), we cannot make any statement. The second line of Eq. (9) asserts that states of the up cluster that lie above the initial state will finally be unpopulated. This no-go theorem was formulated in Refs. 56 and 57 and we think that it is more aptly described by the name “no-go-up theorem.”

A case of particular interest is that of the initial state $|\uparrow 0_+\rangle$, which is the ground state of the entire system. For all bath models employed below, the ground state is unique, so that relation (9) applies. Then, final states with $k'_+ < k_+$ do not exist, while the occupation of final states with $k'_+ > k_+$ is forbidden by the no-go-up theorem. Thus, provided that the final qubit state is $|\uparrow\rangle$, the environment will end up in its ground state.

It is the final transition probabilities $P_{\uparrow \rightarrow \uparrow}$ and $P_{\uparrow \rightarrow \downarrow}$ for the qubit that interest us most, irrespective of the final state of the environment. By tracing out the environment, i.e., by performing the sum over k'_+ , we find

$$P_{\uparrow \rightarrow \uparrow} = \exp\left(-\frac{\pi W^2}{2\hbar v}\right) = 1 - P_{\uparrow \rightarrow \downarrow}, \quad (10)$$

with the ground-state expectation value

$$W^2 = 4\langle \uparrow 0_+ | \mathcal{V}^2 | \uparrow 0_+ \rangle. \quad (11)$$

These are the two central equations for dissipative Landau-Zener transitions at zero temperature. The ground-state expectation value W^2 formally replaces the squared tunnel matrix element Δ^2 in the original Landau-Zener expression [Eq. (2)].

III. DISSIPATIVE LANDAU-ZENER TRANSITIONS IN VARIOUS ENVIRONMENTS

We are now in the position to study Landau-Zener transitions for specific baths with linear couplings to the qubit. We will focus on the two most important bath models in quantum dissipation, namely, a bath of harmonic oscillators and a spin bath. In both cases, we will restrict ourselves to zero temperature, so that the natural initial state is the diabatic ground state $|\uparrow 0_+\rangle$ of the system plus the environment. Both for the harmonic-oscillator bath and for the spin bath, the ground state is nondegenerate, so that formula (10) can be applied. The essential steps that remain are first to identify and characterize the diabatic ground state $|\uparrow 0_+\rangle$ and then to compute the expectation value (11). Applications to specific experiments will be discussed in Sec. V.

A. Harmonic-oscillator bath

We first consider the case in which a qubit interacts with a standard bosonic bath consisting of harmonic oscillators. The Hamiltonian is as in Eq. (3), with the environment Hamiltonian

$$\mathcal{H}_{\text{env}} = \sum_{j=1}^N \hbar \Omega_j b_j^\dagger b_j \quad (12)$$

consisting of N harmonic oscillators with frequencies Ω_j . Zero-point energies do not play a role here and are ignored. The b_j^\dagger and b_j denote the usual creation and annihilation operators of the oscillator j . We leave the number of oscillators N finite at first but eventually take it to infinity in a continuum limit. Furthermore, we assume the most general linear qubit-oscillator coupling

$$\mathcal{H}_{\text{q-env}} = \sum_{\nu=x,y,z} \sigma_\nu \sum_{j=1}^N \frac{\gamma_j}{2} \lambda_j^\nu (b_j + b_j^\dagger), \quad (13)$$

where the second sum specifies the environment operators \mathcal{X}^ν defined in Eq. (4). Since the coupling (13) also includes the σ_y interaction, this constitutes a generalization of the spin-boson model that we considered in Ref. 38. The parameters γ_j determine the coupling strengths, while the parameters λ_j^ν define the ‘‘coupling directions’’ and are conveniently expressed by the spherical coordinates ϑ_j and φ_j as

$$\lambda_j^x = \sin \vartheta_j \cos \varphi_j, \quad (14a)$$

$$\lambda_j^y = \sin \vartheta_j \sin \varphi_j, \quad (14b)$$

$$\lambda_j^z = \cos \vartheta_j. \quad (14c)$$

The bit-flip interaction (7) then becomes

$$\mathcal{V} = \frac{\Delta}{2} \sigma_x + \sum_{j=1}^N \frac{\gamma_j \sin \vartheta_j}{2} (\sigma_x \cos \varphi_j + \sigma_y \sin \varphi_j) (b_j + b_j^\dagger). \quad (15)$$

The diabatic states of the environment are determined by diagonalizing the Hamiltonian

$$\mathcal{H}_{\text{env}} + \mathcal{X}^z = \sum_j \hbar \Omega_j b_j^\dagger b_j + \sum_j \frac{\gamma_j}{2} \cos \vartheta_j (b_j^\dagger + b_j) \quad (16)$$

$$= \sum_j \hbar \Omega_j b_{j+}^\dagger b_{j+} - \sum_j E_j. \quad (17)$$

In order to obtain the diagonal form in the last line, we introduced the shifted annihilation operators

$$b_{j+} = b_j + \frac{\gamma_j \cos \vartheta_j}{2\hbar \Omega_j} \quad (18)$$

and the reorganization energy of the j th oscillator, $E_j = (\gamma^2/4\hbar \Omega_j) \cos^2 \vartheta_j$. The latter quantity denotes the energy shift of the oscillator ground state owing to the coupling to the qubit. From Eq. (17), it becomes immediately clear that the diabatic ground state has to fulfill the relation

$$b_{j+} |\uparrow 0_+\rangle = 0, \quad (19)$$

while the excited diabatic states are created by applying the operators b_{j+}^\dagger to this diabatic ground state.

We now write the bit-flip interaction \mathcal{V} with the shifted operators b_{j+} and employ relation (19) to evaluate the ground-state expectation value (11). After some algebra, we obtain³⁸

$$W^2 = \left| \Delta - \sum_j \frac{\gamma_j^2 \sin(2\vartheta_j) e^{-i\varphi_j}}{2\hbar \Omega_j} \right|^2 + \sum_j \gamma_j^2 \sin^2 \vartheta_j, \quad (20)$$

which allows one to compute the Landau-Zener transition probabilities (10). Note the φ_j dependence, generalizing our recent work,³⁸ which shows that for $\Delta \neq 0$, it makes a difference for Landau-Zener transition probabilities what types of off-diagonal qubit-oscillator couplings exist.

Identical coupling angles

For system-bath models, it is frequently assumed that all bath oscillators couple to the central quantum system via the same coordinate. In our model, this corresponds to the case in which all coupling angles are identical, $\vartheta_j = \vartheta$ and $\varphi_j = \varphi$. Then, Eq. (20) becomes

$$W^2(\vartheta, \varphi) = \left| \Delta - \frac{1}{2} E_0 \sin(2\vartheta) e^{-i\varphi} \right|^2 + S \sin^2 \vartheta, \quad (21)$$

in terms of the integrated spectral density⁵⁸

$$S = \sum_j \gamma_j^2 = \frac{\hbar^2}{4\pi} \int_0^\infty d\omega J(\omega) \quad (22)$$

and the energy

$$E_0 = \sum_j \frac{\gamma_j^2}{\hbar\Omega_j} = \frac{\hbar}{4\pi} \int_0^\infty d\omega \frac{J(\omega)}{\omega}, \quad (23)$$

which equals four times the total reorganization energy $E = \sum_j E_j$. These quantities S and E_0 were presented as frequency integrals over the spectral density $J(\omega)$ of the bath, with the latter defined as

$$J(\omega) = \pi \sum_{j=1}^N \left(\frac{2\gamma_j}{\hbar} \right)^2 \delta(\omega - \Omega_j). \quad (24)$$

In a continuum limit, the spectral density becomes a smooth function of frequency. At low frequencies, one typically observes a power-law behavior for $J(\omega)$, whereas the qubit becomes insensitive to high frequencies, as characterized by a cutoff frequency ω_c . An important class of spectral densities is therefore^{31,34}

$$J(\omega) = \alpha \omega^s e^{-\omega/\omega_c}. \quad (25)$$

For such spectral densities, one immediately obtains the two global quantities whereby the bath influences LZ transition probabilities:

$$S = \frac{\alpha \hbar^2}{4\pi} \omega_c^{s+1} \Gamma(s+1), \quad (26)$$

$$E_0 = \frac{\alpha \hbar}{4\pi} \omega_c^s \Gamma(s), \quad (27)$$

where $\Gamma(x)$ denotes the Euler gamma function.

(a) *Off-diagonal coupling.* For $\vartheta = \pi/2$, the qubit interacts via its off-diagonal operators σ_x and σ_y with the environment, whereas the LZ driving affects the qubit only via σ_z . Equation (21) becomes

$$W^2(\pi/2, \varphi) = \Delta^2 + S. \quad (28)$$

Interestingly enough, the Landau-Zener tunneling probability is then fully determined by the integrated spectral density S . In particular, there is no dependence on the oscillator frequencies Ω_j . This result is nicely illustrated in the simple example of Fig. 3, showing Landau-Zener dynamics of a qubit that is coupled to only three oscillators. The oscillator frequencies are varied, while the qubit-oscillator couplings are kept constant. The dynamics at intermediate times depends on the oscillator frequencies, but the final transition probability does not.

Note that $W^2(\pi/2, \varphi)$ in Eq. (28) is independent of φ , so that in case of *only off-diagonal coupling*, the relative weight of the interactions via σ_x and σ_y drops out of the final occupation probability. Since $S > 0$, it is clear from Eqs. (11) and (28) that an off-diagonal coupling always enhances the occupation of the final ground state $|\downarrow\rangle$ as compared to the case without dissipation. This has an intuitive explanation: the zero-temperature oscillator bath partially succeeds in

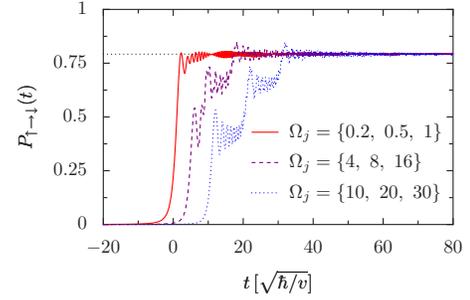


FIG. 3. (Color online) Landau-Zener dynamics for a qubit with $\Delta=0$, in all three cases shown off-diagonally coupled via σ_x to three oscillators. The various oscillator frequencies Ω_j are given in units of $\sqrt{v/\hbar}$. All coupling strengths have the same value $\gamma_j = \sqrt{\hbar v/3}$. The dotted line marks the analytical final transition probability corresponding to Eq. (28).

cooling the qubit down to its instantaneous ground state at any time during the level crossing.

(b) *Diagonal coupling.* For $\vartheta=0$, the qubit interacts with the environment through the diagonal Pauli matrix σ_z . This interaction induces pure dephasing between the states $|\uparrow\rangle$ and $|\downarrow\rangle$. This driven spin-boson model with diagonal interaction has so far been the standard model for discussing Landau-Zener transitions in dissipative environments.^{39,41,44,45,59} For diagonal coupling, the bit-flip interaction (15) simply becomes $\mathcal{V} = (\Delta/2)\sigma_x$, so that

$$W(0, \varphi)^2 = \Delta^2, \quad (29)$$

and the Landau-Zener transition probability (10) coincides with the standard expression (2) for an isolated qubit. This bath independence of the transition probability for diagonal coupling was predicted by Ao and Rammer in the limits of fast and slow Landau-Zener sweeps.³⁹ Here, we find that at zero temperature, it holds exactly for all diagonally coupled harmonic-oscillator baths and for all coupling strengths Δ and sweep velocities v .³⁸

(c) *General coupling.* When the oscillators neither couple purely off diagonally ($\vartheta = \pi/2$) nor purely diagonally ($\vartheta = 0$), the Landau-Zener probability generally exhibits a non-monotonic dependence on the tunnel coupling Δ . This is shown in Fig. 4 for various angles φ and ϑ . Most interesting is the comparison to the nondissipative case, which, as we saw, coincides with the result for diagonal coupling ($\vartheta=0$): Any dissipative Landau-Zener probability lower than the curve for $\vartheta=0$ is counterintuitive. Such situations do occur: for several values of ϑ and for a sufficiently large tunnel splitting Δ , the bath coupling reduces $P_{\uparrow \rightarrow \downarrow}(\infty)$, i.e., dissipation enhances the population of the final excited qubit state.³⁸

This counterintuitive behavior is most significant for the angles $\varphi=0$ and $\vartheta=\pi/4$ and when the squared reorganization energy is large compared to the integrated spectral density $E_0^2 \gg S$. This means that the counterintuitive behavior would be observable only in rather exceptional situations, which did not shape our intuition. For example, for the spectral density (25), a significant reduction of the ground-state population by increase of Δ requires a very strong qubit-bath coupling $\alpha \geq 1$. In the opposite limit $\alpha \ll 1$, which is relevant

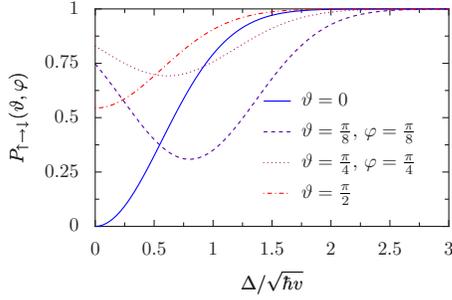


FIG. 4. (Color online) Transition probability $P_{\uparrow \rightarrow \downarrow}$ as a function of the internal coupling Δ for $E_0 = 2\sqrt{\hbar v}$ and $S = 0.5\hbar v$. The angles $\vartheta = 0$ and $\vartheta = \pi/2$ correspond to purely diagonal and off-diagonal couplings, respectively, for which the probability is independent of φ .

for quantum information processing, the bath for all practical purposes induces the more intuitive tendency toward the ground state as Δ is increased, as we found above for purely off-diagonal or purely diagonal couplings.

B. Spin bath

Let us now turn to the case in which a qubit interacts with an ensemble of otherwise noninteracting two-level systems forming a spin bath.^{35–37} The total Hamiltonian is again assumed to be of the general form (3), with the standard Landau-Zener Hamiltonian (1) for the qubit, but now with the bath Hamiltonian

$$\mathcal{H}_{\text{env}} = \sum_{j=1}^N \sum_{\nu=x,y,z} B_j^\nu \boldsymbol{\tau}_\nu^j, \quad (30)$$

where $\boldsymbol{\tau}_\nu^j$ are the Pauli matrices for the j th bath spin. The most general linear qubit-bath coupling reads

$$\mathcal{H}_{\text{q-env}} = \sum_{\nu=x,y,z} \boldsymbol{\sigma}_\nu \sum_{j=1}^N \gamma_j^\nu \boldsymbol{\tau}_\nu^j, \quad (31)$$

where the second sum defines the operators \mathcal{X}^ν as a linear combination of the spin operators $\boldsymbol{\tau}_\nu^j$, with coupling constants γ_j^ν . The bit-flip interaction \mathcal{V} then becomes

$$\mathcal{V} = \frac{\Delta}{2} \boldsymbol{\sigma}_x + \sum_{j=1}^N (\gamma_j^x \boldsymbol{\sigma}_x \boldsymbol{\tau}_x^j + \gamma_j^y \boldsymbol{\sigma}_y \boldsymbol{\tau}_y^j). \quad (32)$$

As for the bosonic bath in Sec. III A, we wish to apply the general formula (10) for the transition probability. For that, we need to determine the diabatic eigenstates of the qubit plus the spin bath. For large $|t|$, the time-dependent term $vt\boldsymbol{\sigma}_z/2$ dominates and, therefore, provides the diabatic qubit states $|\uparrow\rangle$ and $|\downarrow\rangle$. Consequently, the diabatic spin-bath states are determined by the operator

$$\langle s | \mathcal{H}(t) | s \rangle = \sum_j \mathcal{H}_{\text{spin},j}^\pm, \quad s = \uparrow, \downarrow, \quad (33)$$

where “+” refers to $s = \uparrow$ and “−” to $s = \downarrow$, while

$$\mathcal{H}_{\text{spin},j}^\pm = \pm \gamma_j^z \boldsymbol{\tau}_z^j + \sum_{\nu=x,y,z} B_j^\nu \boldsymbol{\tau}_\nu^j \quad (34)$$

determines the state of the j th bath spin. The Hamiltonian (34) is readily diagonalized and its eigenenergies $-\Lambda_{j,\pm}$ and $\Lambda_{j,\pm}$ are determined by

$$\Lambda_{j,\pm} = \sqrt{(B_j^x)^2 + (B_j^y)^2 + (B_j^z \pm \gamma_j^z)^2}. \quad (35)$$

For the evaluation of the Landau-Zener transition probability, we will not need an explicit expression for the ground states $|0_{j,\pm}\rangle$ of $\mathcal{H}_{\text{spin},j}^\pm$. It suffices to know that the ground states satisfy the eigenvalue equation $\mathcal{H}_{\text{spin},j}^\pm |0_{j,\pm}\rangle = -\Lambda_{j,\pm} |0_{j,\pm}\rangle$. Consequently,

$$\langle 0_{j+} | \boldsymbol{\tau}_x^j | 0_{j+} \rangle = -B_j^x / \Lambda_{j+}, \quad (36a)$$

$$\langle 0_{j+} | \boldsymbol{\tau}_y^j | 0_{j+} \rangle = -B_j^y / \Lambda_{j+}, \quad (36b)$$

$$\langle 0_{j+} | \boldsymbol{\tau}_z^j | 0_{j+} \rangle = -(B_j^z + \gamma_j^z) / \Lambda_{j+}. \quad (36c)$$

Since the bath spins do not interact with each other, the diabatic ground state $|0_\pm\rangle$ is the direct product of the states $|0_{j,\pm}\rangle$.

With this ground state defined, we are now in the position to employ formula (10). Inserting relations (36) into (11), we obtain

$$\begin{aligned} W^2 = & \Delta^2 - 4\Delta \sum_j (\gamma_j^x)^2 \frac{B_j^x}{\Lambda_{j+}} + 4 \sum_j [(\gamma_j^y)^2 + (\gamma_j^z)^2] \\ & + 4 \sum_{j \neq j'} \left(\gamma_j^x \gamma_{j'}^x \frac{B_j^x B_{j'}^x}{\Lambda_{j+} \Lambda_{j'+}} + \gamma_j^y \gamma_{j'}^y \frac{B_j^y B_{j'}^y}{\Lambda_{j+} \Lambda_{j'+}} \right) \\ & + 8 \sum_j \gamma_j^x \gamma_j^y \frac{B_j^z}{\Lambda_{j+}}, \end{aligned} \quad (37)$$

which determines the Landau-Zener transition probability (10). The last term stems from the commutator $[\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y] = 2i\boldsymbol{\sigma}_z$. Recall that the general Landau-Zener formula (10) was derived under the assumption that the diabatic qubit-plus-bath ground state at $t = -\infty$ is nondegenerate. Therefore, our results do not apply to parameter sets for which any bath spin obeys $B_j^x = B_j^y = (B_j^z + \gamma_j^z) = 0$ so that $\Lambda_{j+} = 0$.

(a) *Diagonal basis for spins.* First, we consider the physically important special case that all B_j^x and B_j^y vanish, so that the eigenvalues become $\Lambda_{j+} = |B_j^z + \gamma_j^z|$. The ground-state expectation value W^2 which determines the tunnel rate then assumes the more compact form

$$W^2 = \Delta^2 + 4 \sum_{j=1}^N (\gamma_j^x + s_j \gamma_j^y)^2, \quad (38)$$

where $s_j \equiv \text{sgn}(B_j^z + \gamma_j^z)$. We can see that in this special case, the transition probability is independent of the eigenfrequencies Λ_j/\hbar ; the probability essentially depends on the qubit-spin coupling strengths γ_j^ν . This frequency independence resembles the transition probability (28) for the off-diagonally coupled bosonic oscillator bath, although the qubit-spin coupling in the present case is not necessarily off diagonal.

(b) *Pure dephasing.* Interestingly, it follows from Eq. (38)

that if all $(\gamma_j^x + s_j \gamma_j^y)$ vanish, then the tunneling probability $P_{\uparrow \rightarrow \downarrow}$ equals the standard LZ probability (2), despite the coupling to the bath. This includes the important case of pure diagonal coupling for which $\gamma_j^x = \gamma_j^y = 0$. This bath independence confirms and generalizes the very recent perturbative calculations by Wan *et al.*⁶⁰ for dissipative LZ transitions in a spin bath, where it was assumed that Δ is small. We find the same exact bath-independent transition probability in case of a diagonally coupled spin bath as we found earlier in Sec. III A for a diagonally coupled bosonic bath. This striking result is discussed further in Sec. IV.

(c) *Robustness under dephasing.* Without loss of generality, the energies B_j^z of the spins can be chosen positive. For spin baths away from the very strong coupling regime, the coupling constants γ_j^z will be much smaller than the corresponding energies B_j^z , so that $\text{sgn}(B_j^z + \gamma_j^z) = 1$. Thus, unless the qubit-spin coupling is very strong, the LZ transition probability corresponding to Eq. (38) is independent of the γ_j^z . Interestingly, we find that this holds true even when $\gamma_j^z \gg \gamma_j^{x,y}$, i.e., if dephasing is much stronger than relaxation.

Moreover, in many models for decoherence by spin baths, the coupling of the bath to the σ^y operator simply does not occur, in which case Eq. (38) reduces to

$$W^2 = \Delta^2 + 4 \sum_{j=1}^N (\gamma_j^x)^2. \quad (39)$$

Note that this result is obtained without making any assumptions on the dephasing strengths γ_j^z . In other words, the LZ transition probability only depends on the integrated spectral density for relaxation and is *fully independent* of the dephasing strength of the spin bath. As discussed in Sec. V, this is important in experiments.

IV. UNIVERSALITY OF BATH-INDEPENDENT NONADIABATIC TUNNELING PROBABILITY

As was found in the previous section, when the qubit interacts with a bosonic bath or with a spin bath only via the operator σ_z and the total system starts in its ground state, then the probabilities for dissipative Landau-Zener transitions coincide with the standard tunneling probability (2). Thus, a natural question arises: Is this a coincidence, a specialty of the two baths that we studied, or does it hold more generally? We will now show that this holds in general, regardless of the specifics of the environment. Consider the Hamiltonian

$$\mathcal{H} = \frac{vt}{2} \sigma_z + \frac{\Delta}{2} \sigma_x + \sigma_z \mathcal{X} + \mathcal{H}_{\text{env}}, \quad (40)$$

which is the general Hamiltonian (3) specified for diagonal coupling ($\lambda^x = \lambda^y = 0$). As before in Sec. II B, the operator \mathcal{X} is the environment operator with which the environment is coupled to the qubit, and \mathcal{H}_{env} is the environment Hamiltonian. Further specifications of these operators need not be given for our reasoning. Note that the qubit-bath interaction $\sigma_z \mathcal{X}$ does not commute with the standard LZ Hamiltonian at any time if $\Delta \neq 0$. Taking this at face value, it is tempting to

assume that the transition probability $P_{\uparrow \rightarrow \downarrow}$ will be affected by a bath that causes pure dephasing. Our analysis, however, will reveal that this is not the case.

As before, a complete set of diabatic qubit-plus-bath states $|\uparrow k_+\rangle$ and $|\downarrow k_-\rangle$ can be found, where the shifted diabatic bath states $|k_{\pm}\rangle$ are eigenstates of $(\mathcal{H}_{\text{env}} \pm \mathcal{X}^z)$. We assume that $(\mathcal{H}_{\text{env}} + \mathcal{X}^z)$ has a nondegenerate ground state $|0_+\rangle$. Now, since the bath does not induce bit flips, the bit-flip operator (7) simply reduces to the *internal* bit-flip interaction, i.e., $\mathcal{V} = \Delta \sigma_x / 2$. Hence, $W^2 = \Delta^2$. Thus, from (10), we find the standard Landau-Zener transition probability for a qubit diagonally coupled to an arbitrary bath at zero temperature as follows:

$$P_{\uparrow \rightarrow \downarrow} = 1 - \exp\left(-\frac{\pi \Delta^2}{2 \hbar v}\right). \quad (41)$$

It is truly remarkable that diagonal coupling to the environment does not affect the final transition probability, whatever the nature of the environment and however strong the coupling operator \mathcal{X}^z may be. In other words, this zero-temperature transition probability for diagonal bath coupling (41) indeed holds universally. It may have been simple to derive it from Eq. (10), but the physical implications are most important: Landau-Zener transitions are insensitive to pure dephasing at zero temperature, irrespective of the nature of the bath or of the bath-coupling operator \mathcal{X}^z .

To illustrate the universality that we just found, let us now also consider the coupling to a collection of *nonlinear* oscillators,

$$\mathcal{H}_{\text{env}} = \sum_{j=1}^N \hbar \Omega_j b_j^\dagger b_j + \frac{\beta_j}{4!} (b_j^\dagger + b_j)^4, \quad (42)$$

that couples to the qubit via the interaction operator

$$\mathcal{X}^z = \sum_{j=1}^N \frac{\gamma_j}{2} (b_j^\dagger + b_j). \quad (43)$$

LZ sweeps past resonances of nonlinear oscillators are of practical interest, since nonlinear oscillators are currently used for the readout of flux qubits.⁶¹ For a numerical test of the predicted final transition probability, we take the situation in which the qubit is diagonally coupled to two of these nonlinear oscillators. Figure 5 shows the corresponding time evolution of the probability $P_{\uparrow \rightarrow \downarrow}(t)$ for the qubit to be in the “down” state. It also shows the dynamics in case the qubit couples to two linear oscillators with the same parameters, except that now $\beta_{1,2} = 0$. Furthermore, the effect of a diagonally coupled spin bath, a special case of the Hamiltonian (30), is also shown. We consider the case in which the spin bath consists of seven spins. The internal interaction Δ has the same value for all curves in Fig. 5. As shown in the figure, at intermediate times, the transition probability shows variations depending on the specifics of the environments, but the final probabilities indeed all converge to the universal value (41).

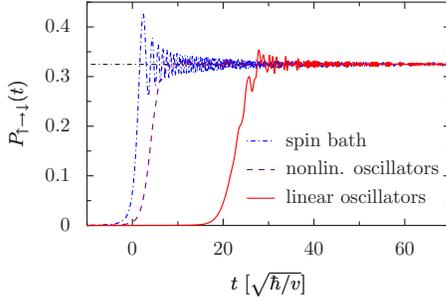


FIG. 5. (Color online) Time evolution of the bit-flip probability for a qubit with $\Delta=0.5\sqrt{\hbar v}$ diagonally coupled to two harmonic oscillators, two nonlinear oscillators, and seven spins, respectively. The harmonic oscillators are specified by $\Omega_1=0.1\sqrt{v/\hbar}$, $\Omega_2=0.5\sqrt{v/\hbar}$, $\gamma_1=2\sqrt{\hbar v}$, and $\gamma_2=6\sqrt{\hbar v}$, while the nonlinear oscillators, in addition, have $\beta_1=\beta_2=3\sqrt{\hbar v}$. The values of the B_j^v and the γ_j^v are randomly chosen from the range $[-\sqrt{\hbar v}/10, \sqrt{\hbar v}/10]$. In all three cases, the transition probability converges to the universal value (41).

V. EXPERIMENTAL RELEVANCE

Landau-Zener transitions are commonly used in experiments to determine the interaction Δ between diabatic energy levels.³ One usually takes the standard LZ formula (2) as a starting point. For fixed sweep speed v of the energy levels, the only unknown in the equation is the internal interaction Δ . By varying v , one can determine the Landau-Zener probability $P_{\uparrow\rightarrow\uparrow}$ and, hence, the Δ . This, in turn, is a method to test the validity of the two-level result (2).

However, if the qubit is coupled to an environment that causes relaxation, then Eq. (28) shows that one actually measures $\sqrt{\Delta^2+S}$ for a qubit in an oscillator bath, where S denotes the integrated spectral density. Variation of the sweep speed v does not help in extracting Δ and S separately from a Landau-Zener experiment. If the bath only couples diagonally and thereby causes only pure dephasing, then at zero temperature, the bath does not influence the Landau-Zener tunneling probability at all.

In most situations, the environment will cause both relaxation and pure dephasing. We find that dephasing will hardly change the relaxation-dependent transition probabilities, see Eqs. (21) and (38). In many experiments pure dephasing is much faster than relaxation; in other words, T_2^* times are much shorter than T_1 times. It will therefore often occur that $S \sin^2 \vartheta \ll \Delta^2$ and, hence, relaxation can be neglected on the time scale of the Landau-Zener transition. Then, our results imply that with a Landau-Zener experiment, one can accurately determine the internal interaction Δ even in the presence of strong dephasing, such that $S \cos^2 \vartheta \gg \Delta^2$. Landau-Zener experiments are therefore a surprisingly reliable tool to determine tunnel splittings. We now consider some specific applications.

A. Circuit QED

Circuit QED (Refs. 62 and 63) is a superconducting-circuit analog of optical cavity QED: A charge qubit⁶² or a flux qubit⁶³ is coupled so strongly to a quantized harmonic

oscillator in the circuit that Rabi oscillations can be observed in a solid-state environment. Because the circuit-QED system is so highly tunable, it enables the study of quantum dynamics of open quantum systems in new parameter regimes. Recently, we proposed using LZ transitions in circuit QED to generate single microwave photons¹⁸ by choosing parameters such that the qubit-oscillator coupling is off-diagonal and the internal interaction Δ vanishes. Here, we consider an arbitrary Δ and discuss the possibility of qubit-oscillator couplings other than off diagonal.

The Hamiltonian describing a charge qubit interacting with the transmission-line resonator is

$$\mathcal{H}(t) = \mathcal{H}_q(t) + \mathcal{H}_{q\text{-osc}} + \mathcal{H}_{\text{osc}}, \quad (44)$$

where the different terms describe the qubit, the oscillator, and the qubit-oscillator coupling, respectively. If the dynamics is essentially restricted to two states with N and $N+1$ Cooper pairs in the box, then the Hamiltonian becomes beautifully simple⁶⁴ and, in our notation, reads

$$\mathcal{H}_q = -\frac{E_J(t)}{2} \sigma_z + \frac{\Delta}{2} \sigma_x, \quad (45a)$$

$$\mathcal{H}_{\text{env}} = \hbar \omega_r \left(b^\dagger b + \frac{1}{2} \right) - \frac{\gamma^2 (1 - 2N_g^{\text{dc}})^2}{\hbar \omega_r}, \quad (45b)$$

$$\mathcal{H}_{q\text{-env}} = \gamma (b + b^\dagger) \sigma_x, \quad (45c)$$

with the oscillator frequency ω_r , and the coupling strength γ . We presented the Hamiltonian in the so-called tunneling representation, which is the basis in which the charge states $|N\rangle$ and $|N+1\rangle$ are eigenstates of σ_x . Since the Josephson link is implemented by a dc superconducting quantum interference device (SQUID), the Josephson energy $E_C(t) = E_{J,\text{max}} \cos[\Phi(t)/\Phi_0]$ can be manipulated upon variation of the flux $\Phi(t)$ that penetrates the SQUID,⁶⁵ where Φ_0 denotes the flux quantum. The dimensionless quantity N_g^{dc} is proportional to an applied gate voltage which can be used to adjust the internal coupling, which, in terms of the control parameters, reads $\Delta = 4(1 - 2N_g^{\text{dc}})(\gamma^2/\hbar \omega_r - E_C)$ with the charging energy E_C .

Since the internal coupling Δ is tunable for this setup, one can use Landau-Zener transitions to determine the integrated spectral density S for the purely off-diagonal coupling (45c). In the one-oscillator model (45), $S = \gamma^2$, so that $W^2 = \Delta^2 + \gamma^2$. Thus, by Landau-Zener sweeps past the oscillator resonance for different values of Δ , Eq. (28) allows one to determine the qubit-oscillator coupling strength γ^2 in independent ways.

The Hamiltonian (45) features a possibly nonzero internal interaction Δ between the qubit levels, which was assumed zero in the setting of this superconducting circuit for which single-photon generation was recently proposed.¹⁸ Besides the transitions $|\uparrow 0\rangle \rightarrow |\downarrow 1\rangle$ that generate a single photon, for $\Delta \neq 0$, there is now also the process $|\uparrow 0\rangle \rightarrow |\downarrow 0\rangle$ which flips the qubit without changing the cavity state. Therefore, a reliable single-photon generation requires that the transitions induced by Δ are not relevant, while the qubit-oscillator coupling has to be sufficiently large,¹⁸ such that $\gamma^2 \gg \hbar v$. Fortu-

nately, as long as $\Delta \ll \hbar \omega_r$, efficient single-photon generation is very well possible by sweeping the qubit energy only on a finite frequency interval small compared to ω_r but large compared to the width of the cavity resonance.

It would be interesting to test in circuit QED our predictions for other than off-diagonal qubit-bath couplings. This requires magnetic fields and gate voltages to be swept simultaneously. The problem with sweeping gate voltages, however, is that this displaces the ground state of the oscillator,⁶⁴ which practically means that Δ cannot be used as a time-dependent control parameter. Consequently, the electric-plus-magnetic sweeping in circuit QED falls outside the class of models that we considered. It seems that Landau-Zener transitions with a general qubit-oscillator coupling angle ϑ as in (15) cannot be engineered in state-of-the-art circuit QED.

We already mentioned the width of the cavity resonance, but actually in the model (45), we assumed that the quality factor of the resonator was infinite. The spectral density of the oscillator bath then consists of a single delta peak at the cavity resonance frequency, so that $S = \gamma^2$. For the nonideal resonance, the spectral density becomes^{25,26}

$$J(\omega) = \frac{\alpha \kappa \omega_r^4 \omega}{(\omega^2 - \omega_r^2)^2 + \kappa^2 \omega_r^2 \omega^2}, \quad (46)$$

where the dimensionless parameters α and κ measure the qubit-oscillator strength and the width of the resonance peak, respectively. For small frequencies $\omega \ll \omega_r$, the spectral density $J(\omega) \approx \alpha \kappa \omega$, as for an Ohmic bath. Now, suppose that we let the qubit undergo a LZ sweep from frequency zero across the resonator frequency until a frequency $\omega_{\max} > (1 + \kappa) \omega_r$. Now, since for frequencies $|\omega - \omega_r| > \kappa \omega_r$ the spectral density falls off rapidly, a hypothetical continuation of the LZ sweep from frequency ω_{\max} to infinity would hardly change the transition probability. Therefore, by combining (22) and (46), we find the integrated spectral density

$$S = \frac{\alpha (\hbar \omega_r)^2}{4\pi} \left[\arctan\left(\frac{2 - \kappa^2}{\kappa \sqrt{4 - \kappa^2}}\right) + \frac{\pi}{2} \right] \approx \frac{\alpha (\hbar \omega_r)^2}{4}. \quad (47)$$

Inserting this expression into (28) gives an accurate value for the cavity-induced LZ transition probability. The last identity in (47) holds in the experimentally realized good-cavity limit $\kappa \ll 1$. In this limit, one can approximate the spectral density (46) by a single oscillator with qubit-oscillator coupling $\gamma^2 = \alpha (\hbar \omega_r)^2 / 4$, reproducing the model (45).

This leads us to the important conclusion that LZ transition probabilities can be computed exactly for qubits swept past narrow or broad cavity resonances alike. The total strength S of the atom-cavity coupling determines the LZ transition probability, and for weak dissipation, S is independent of the scaled cavity width κ . Dissipative Landau-Zener transitions are also robust in this respect.

B. Cavity QED and photonic crystals

Atoms couple off diagonally to the electromagnetic field, which, for many practical purposes, can be considered as a bath at zero temperature. Atomic energies can be swept by

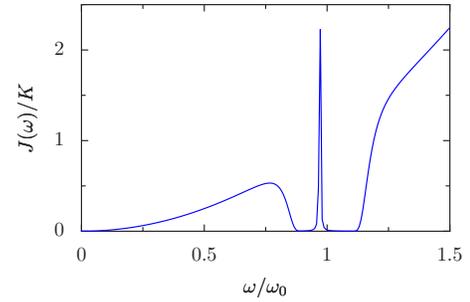


FIG. 6. (Color online) Sketch of spectral density for an atom near a local defect in a photonic crystal with a band gap. The quadratic free-space spectral density is modified by the crystal that creates a spectral gap around ω_0 . A narrow defect mode inside a broader band gap allows a controlled atom-defect interaction via LZ sweeps of the atomic transition frequency $\omega_A(t)$.

applying dc electric and magnetic fields, which give rise to Stark and Zeeman shifts, respectively. Atomic resonances are usually narrow but hard to sweep by large percentages. Artificial atoms are more tunable, but their resonances are also broader. Our results apply to situations where resonances can be swept by much more than their width.

An atom in free space feels a spectral density that is quadratic in the frequency, $J(\omega) \propto (\omega/\omega_0)^2$, with no cutoff frequencies in the optical regime, so that $S \rightarrow \infty$. During a Landau-Zener sweep of an atom in free space, the atom will finally have decayed spontaneously to its ground state. However, the spectral density felt by the atom, also known as its local optical density of states,⁶⁶ can be engineered by changing its dielectric environment. In photonic crystals, for example, the periodicity of the refractive index on the scale of an optical wavelength $\lambda_0 = 2\pi c/\omega_0$ may create a photonic band gap. Within this gap, the spectral density $J(\omega)$ ideally vanishes and, in practice, it can be strongly reduced, whereby spontaneous emission by the atom is strongly suppressed.⁶⁷

By making a controlled point defect or line defect in the vicinity of the atom that breaks the periodicity of the photonic crystal, a narrow defect mode may be created⁶⁸ within the spectral gap, as sketched in Fig. 6. Ideally, this would allow cavity QED experiments to be performed within a photonic crystal, and progress is made in this direction.^{67,68} We propose to do LZ sweeps of the atomic frequency $\omega_A(t)$ around the defect frequency but within the band gap. This will allow the creation of atom-defect entanglement and of single photons in the defect mode, in quite the same way as in circuit QED.¹⁸

C. Molecular nanomagnets

The energy levels of molecular nanomagnets can be swept by switching on dc magnetic fields.³ Higher excited states have higher magnetization, and these are excited more when switching rates are high. These nanomagnets are not intrinsic two-level systems, and indeed many successive LZ transitions are observed upon increasing the magnetic field. They can be cooled until tunneling rates become temperature independent.³ In recent experiments,⁴ this happens rather

abruptly at a temperature of 0.6 K. In this low-temperature pure quantum tunneling regime, our predictions apply. LZ transitions are commonly used in experiments to determine level interactions between energy levels of molecular nanomagnets. Energy relaxation due to thermal environment usually changes the effective energy gap.⁶⁹ However, as we showed, LZ transitions for qubits are robust under dephasing, which, on a qualitative level, agrees with previous laboratory experience about LZ transitions in nanomagnets.³

Molecular nanomagnets show many avoided crossings as the magnetic field is varied. These crossings are often well separated, so that one can ask what type of bath influences the effective two-level dynamics around a particular level crossing. Neither the bath nor its coupling to the qubit is known precisely, but at very low temperatures, the main source of decoherence will stem from the coupling to other electronic and nuclear spins, so that a spin bath seems the appropriate model. Our results of Sec. III B show in detail how transition probabilities depend on both the internal interaction Δ and the integrated spectral density S . Although strong dephasing is probable in nanomagnets, our analytical results prove that this hardly affects the LZ transition probabilities in the experimentally accessible regime where tunneling rates are temperature independent.⁴

A theory for *multiple* dissipative LZ transitions in molecular magnets was developed by Leuenerger and Loss.⁷⁰ This theory presumes that in between successive LZ transitions, all quantum coherences have been washed out due to dephasing while dephasing *during* the individual LZ transitions does not influence the transition probabilities. This assumption is rather natural if the LZ tunneling time τ_{LZ} is much shorter than the pure dephasing time, but obviously requires proof for slower LZ transitions. This is an important application of our results: our derivation of the universal bath independence of individual LZ transitions under dephasing proves that the theory of Ref. 70 is more widely applicable than one would have guessed previously.

D. Quantum computer as a spin-bath simulator

An ideal quantum computer is a collection of qubits whose energies and internal interactions are tunable and whose mutual interactions are tunable as well. One method for single-qubit manipulation is a Landau-Zener sweep. This has been realized in recent experiments on superconducting qubits.^{13,17,20} If the interactions with the other qubits are not exactly zero, then our spin-bath result (37) predicts an effect on the “single-qubit” LZ transition probability. In this way, the LZ sweep provides a test of the settings of the quantum computer in the operational space of the qubit.

On the other hand, our predictions can be tested very carefully by controlled variation of qubit-qubit interactions in the quantum computer. Indeed, the quantum computer could be seen as a quantum simulator, in our case of the effects of a spin bath on the LZ transition probability. A full-fledged quantum simulator does not exist yet, but recent experiments on a system of four superconducting qubits with tunable couplings look promising.⁷¹

E. Superconducting qubits and their spin baths

Josephson phase qubits at very low temperatures (20 mK) exhibit decoherence mainly due to interactions with two-

level microwave resonators.²⁷ Since it is found that qubit losses strongly depend on driving amplitudes, these resonators cannot be described as a bosonic bath. Rather, they are nowadays thought to be charge two-level systems.²⁹ The existence of these resonators has important implications for the operation of superconducting qubits. Spectroscopic measurements have shown that at fixed energy, the qubit often resonantly interacts with only a single resonator. Moreover, coherent quantum oscillations between a qubit and such a single resonator were observed.²⁸ Remarkably, decoherence times of these microscopic two-level systems are larger than that of the qubit. This, in turn, has led to the very recent proposal to use instead these microscopic resonators as qubits for quantum information processing.⁷²

Our exact result (37) for the Landau-Zener transition probability of a qubit in a spin bath in the low-temperature tunneling regime can be an important tool for analyzing further the properties of the microscopic resonators and their couplings to the qubit. Our assumption of a spin-star configuration, i.e., a bath of mutually noninteracting spins, is probably correct for the spin bath of the phase qubits.⁷² Monte Carlo simulations indicate that narrower qubit-spin resonances are shadowed by larger ones.²⁹ For that reason, it is important that formula (37) holds generally, whether the qubit resonantly interacts with one microwave resonator at a time or not.

During a so-called fast-pulse measurement of the state of the qubit, the qubit energy moves in and out of resonance with many of these resonators.²⁸ As a consequence, the resonators reduce the fidelity of the measurement. Actually, this effect of the fluctuators has already been estimated in terms of multiple LZ transitions in Ref. 28. There, it was assumed that the resonators couple off diagonally via $\sum_{j=1}^N \gamma_j^x \sigma_x^j$, with coupling strengths $(\gamma_j^x)^2$ given by the size of the splittings as measured in the qubit spectroscopy. Our results (37) and especially (39) show that the formula used in Ref. 28 becomes exact for a zero-temperature spin bath that couples off diagonally, even in the case of overlapping spurious resonances.²⁹ It is unfortunate that microscopic resonators reduce the fidelity of the fast-pulse readout method, but it is good to know how much. More good news is that the same fidelity reduction would be obtained even if there would be additional dephasing by the spins.

Landau-Zener sweeps for phase qubits can be relevant for one more reason:³⁸ the precise spectral distribution of the spins will be sample dependent. Moreover, the distribution for a single sample varies on a time scale of days.⁷² Fortunately, the LZ sweep measures a “global” property of the spin bath, namely, its integrated spectral density S . It is fair to assume that S will vary less from sample to sample and from one day to the next than $J(\omega)$ at a fixed frequency. We therefore suggest using LZ sweeps as a robust way of “gauging” and characterizing the spin-bath environment of superconducting phase qubits.

VI. SUMMARY AND CONCLUSIONS

We studied the effect of various zero-temperature environments on the Landau-Zener transition probability of a qu-

bit. The main result of this paper is the corresponding generalization of the bit-flip probability. The mathematical form of this result, just like the standard Landau-Zener formula, is charmingly simple: from the total Hamiltonian, one identifies the bit-flip operator \mathcal{V} of the qubit and computes the expectation value $W^2 = 4\langle \mathcal{V}^2 \rangle$ for the initial diabatic ground state of the qubit plus its environment. The transition probability follows formally by replacing in the standard expression for the two-level LZ problem the factor Δ^2 by W^2 . Following this recipe, we have calculated in Sec. III the LZ tunneling probabilities for oscillator baths and for spin baths, which represent the two most important environments in quantum dissipation research. These examples illustrated that dissipative Landau-Zener transition probabilities, in general, depend on the type of environment and on the way the qubit couples to it.

However, when the qubit-bath coupling is of the diagonal type, causing so-called pure dephasing, then the tunneling probability coincides with the original LZ probability, regardless of the details of the environment. We expect that this universal behavior is observable and important for a wide variety of applications. A bath independence of another kind was found for a qubit swept past a broadened (circuit) cavity resonance: the transition probability turned out to be independent of the quality factor of the cavity. Since transition probabilities are also independent of the environment parameters in some phenomenological models with non-Hermitian dynamics,^{73,74} possible mappings between these and our models deserve future studies.

For the experimentally important hybrid situation in which the bath causes both relaxation and dephasing, it was found that the influence of dephasing is negligible, unless the qubit-bath coupling is exceptionally strong. This robustness of the LZ transition probability under dephasing is quite surprising and important in applications. Furthermore, the application of our results to experiments in superconducting circuits seems very promising, for example, for circuit QED and for the fast-pulse readout of phase qubits.

In the future, it will be interesting to clarify whether a degeneracy of the ground state modifies the results. The effects of finite temperatures on the LZ tunneling would also deserve thorough investigations in the light of the exact zero-temperature results, with the recent work by Pokrovsky and Sun⁴³ as an important first step. Other experimentally relevant issues are how nonlinear sweeping and finite sweeping times affect the dissipative transition.

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APPENDIX: LANDAU-ZENER TRANSITION IN A MULTILEVEL SYSTEM

We consider the multilevel Hamiltonian

$$H(t) = \sum_a \varepsilon_a |a\rangle\langle a| + \sum_b (\varepsilon_b - v_b t) |b\rangle\langle b| + \sum_{a,b} (X_{ab} |a\rangle\langle b| + X_{ab}^* |b\rangle\langle a|) \quad (\text{A1})$$

with the time-dependent diabatic energies sketched in Fig. 7. We assume that all diabatic states $|a\rangle$, $|b\rangle$ are mutually orthogonal and that all $v_b > 0$. In the limit $t \rightarrow \pm\infty$, the states $|a\rangle$, $|b\rangle$ become eigenstates of the Hamiltonian (A1). The off-diagonal part of the Hamiltonian is such that it only couples states of different groups while states within one group are uncoupled. Without loss of generality, we assumed in the Hamiltonian (A1) that the diabatic energies of the a states are time independent. If they all had an identical velocity v_a smaller than all v_b , we could obtain the Hamiltonian (A1) by a gauge transformation with the time-dependent phase factor $\exp(-iv_a t^2/2\hbar)$. Then, v_b becomes the velocity of the b states with respect to v_a .

We choose as an initial condition that the system starts at $t = -\infty$ in one particular state $|a\rangle$. The central quantity of interest is the probability $P_{a \rightarrow a'}$ for a nonadiabatic Landau-Zener transition to a state $|a'\rangle$ at $t = \infty$.

It is convenient to work in an interaction picture with respect to the diagonal part of the Hamiltonian (A1) and, thus, to apply the unitary transformation

$$U_0(t) = \sum_a e^{-i\varepsilon_a t/\hbar} |a\rangle\langle a| + \sum_b e^{-i\varepsilon_b t/\hbar + iv_b t^2/2\hbar} |b\rangle\langle b|. \quad (\text{A2})$$

Then, we have to deal with the interaction-picture Hamiltonian

$$\tilde{H}(t) = \sum_{a,b} e^{i(\varepsilon_a - \varepsilon_b)t/\hbar + iv_b t^2/2\hbar} X_{ab} |a\rangle\langle b| + \text{H.c.} \quad (\text{A3})$$

In the interaction representation, the nonadiabatic transition probability reads

$$P_{a \rightarrow a'} = |\langle a' | S | a \rangle|^2, \quad (\text{A4})$$

where the S matrix is given by the usual time-ordered exponential

$$S = \sum_{k=0}^{\infty} \left(-\frac{i}{\hbar} \right)^{2k} S_k, \quad (\text{A5})$$

with the $2k$ th-order contribution

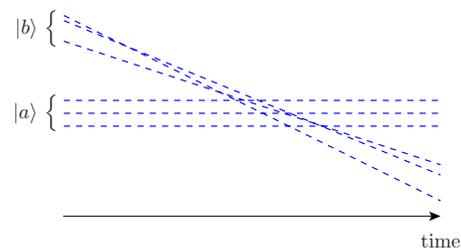


FIG. 7. (Color online) Crossing of two groups of diabatic states: states $|a\rangle$ whose energy is time independent and states $|b\rangle$ whose energies are reduced with constant velocities v_b .

$$S_k = \int_{-\infty}^{\infty} dt_1 \int_{t_1}^{\infty} dt_2 \cdots \int_{t_{2k-1}}^{\infty} dt_{2k} \tilde{H}(t_{2k}) \cdots \tilde{H}(t_1). \quad (\text{A6})$$

Note that the interaction-picture Hamiltonian $\tilde{H}(t)$ always flips between states $|a\rangle$ and $|b\rangle$, so that the perturbation series for the transition amplitude in (A4) only consists of even powers of the interaction X_{ab} .

In order to compute the matrix element $\langle a' | S_k | a \rangle$, we will generalize and simplify our reasoning of Refs. 18 and 38 for this more general model. To begin with, we insert $2k-1$ times the unit operator $\sum_a |a\rangle \langle a| + \sum_b |b\rangle \langle b|$ and obtain

$$\begin{aligned} & \sum_{a_1 \cdots a_{k-1}} \sum_{b_1 \cdots b_k} X_{a'b_k} X_{a_{k-1}b_k}^* X_{a_{k-1}b_{k-1}} X_{a_{k-1}b_{k-1}}^* \cdots X_{a_1 b_1} X_{ab_1}^* \\ & \times \int_{-\infty}^{\infty} dt_1 \cdots \int_{t_{2k-1}}^{\infty} dt_{2k} \exp \left[\frac{i}{\hbar} (\varepsilon_{b_1} - \varepsilon_a) t_1 \right. \\ & + \frac{i}{\hbar} \sum_{\ell=2}^k (\varepsilon_{b_\ell} - \varepsilon_{a_{\ell-1}}) t_{2\ell-1} + \frac{i}{\hbar} \sum_{\ell=1}^{k-1} (\varepsilon_{a_\ell} - \varepsilon_{b_\ell}) t_{2\ell} \\ & \left. + \frac{i}{\hbar} (\varepsilon_{a'} - \varepsilon_{b_k}) t_{2k} + \frac{i}{2\hbar} \sum_{\ell=1}^k v_{b_\ell} (t_{2\ell}^2 - t_{2\ell-1}^2) \right]. \quad (\text{A7}) \end{aligned}$$

In order to cope with the time ordering, we substitute the time variables t_1, \dots, t_{2k} by the time differences $\tau_\ell = t_{2\ell} - t_{2\ell-1}$ and $u_\ell = t_{2\ell+1} - t_{2\ell}$ as sketched in Fig. 8(a), i.e., we set

$$t_1 = t, \quad (\text{A8a})$$

$$t_{2\ell} = t + \sum_{\ell'=1}^{\ell} \tau_{\ell'} + \sum_{\ell'=1}^{\ell-1} u_{\ell'}, \quad (\text{A8b})$$

$$t_{2\ell+1} = t + \sum_{\ell'=1}^{\ell} (\tau_{\ell'} + u_{\ell'}), \quad (\text{A8c})$$

which is equivalent to $\tau_\ell = t_{2\ell} - t_{2\ell-1}$ and $u_\ell = t_{2\ell+1} - t_{2\ell}$. Note that the Jacobian of this substitution is 1. Then, the multiple time integral in expression (A7) becomes

$$\begin{aligned} & \int_{-\infty}^{\infty} dt \int_0^{\infty} du_1 \cdots du_{k-1} \int_0^{\infty} d\tau_1 \cdots d\tau_k \\ & \times \exp \left[\frac{i}{\hbar} \left(\varepsilon_{a'} - \varepsilon_a + \sum_{\ell=1}^k v_{b_\ell} \tau_\ell \right) t \right. \\ & + \frac{i}{\hbar} \sum_{\ell=1}^k (\varepsilon_{a'} - \varepsilon_{b_\ell}) \tau_\ell + \frac{i}{\hbar} \sum_{\ell=1}^{k-1} (\varepsilon_{a'} - \varepsilon_{a_\ell}) u_\ell \\ & \left. + \frac{i}{\hbar} \sum_{\ell=1}^k \left(\frac{1}{2} v_{b_\ell} \tau_\ell^2 + v_{b_\ell} \tau_\ell \sum_{\ell'=1}^{\ell-1} (\tau_{\ell'} + u_{\ell'}) \right) \right]. \quad (\text{A9}) \end{aligned}$$

Performing the t integration, we obtain the Dirac delta

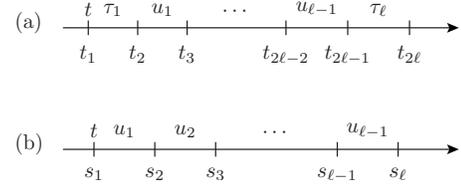


FIG. 8. Relation between the various time variables.

$$2\pi\hbar \delta \left(\varepsilon_{a'} - \varepsilon_a + \sum_{\ell=1}^k v_{b_\ell} \tau_\ell \right). \quad (\text{A10})$$

Because all $v_b > 0$ and the integration interval for each τ_ℓ is $[0, \infty)$, the sum in the argument of the delta function is non-negative. This has two important implications.

First, the energies of the final and the initial state must fulfill the relation $\varepsilon_{a'} \leq \varepsilon_a$, which means that all states $|a'\rangle$ with an adiabatic energy higher than that of the initial state $|a\rangle$ are finally unoccupied, or

$$P_{a \rightarrow a'} = 0 \quad \text{for } \varepsilon_{a'} > \varepsilon_a. \quad (\text{A11})$$

We call this no-go theorem^{55,56} the no-go-up theorem. As a corollary, we find that if the system starts at $t = -\infty$ in the adiabatic ground state, the final state will be either the initial state or one of the states $|b\rangle$.

If all avoided crossings of the adiabatic energies are sufficiently narrow, the no-go-up theorem can be understood by semiclassical considerations: At each avoided crossing, the population splits up into a coherent superposition of two branches. If the system starts out in an a state which has velocity $v_a = 0$, it can only choose between staying in an a state with constant energy or a b state with decreasing energy. Thus, transitions to diabatic states with higher energies are impossible. Note that the validity of these semiclassical arguments is limited while the no-go-up theorem (A11) is an exact statement that holds for any width of the avoided crossings.

The second implication of (A10) concerns the special transitions $|a\rangle \rightarrow |a\rangle$, to which the remainder of this Appendix is devoted. Since in this case the sum in the delta function must vanish, any contribution to the corresponding transition probability must come from the subspace $\tau_1 = \tau_2 = \cdots = \tau_k = 0$. This means that the τ integrals in expression (A9) vanish unless the u integrals are singular for $\tau_\ell = 0$. This finding can be exploited for the simplification of the u integrals. In the present form, however, the twofold summation in the last term of the exponent in expression (A9) will complicate this task. Therefore, it is convenient to substitute the integration variables u_1, \dots, u_{k-1} by the times

$$s_\ell = t + \sum_{\ell'=1}^{\ell-1} u_{\ell'}, \quad (\text{A12})$$

which means $u_\ell = s_{\ell+1} - s_\ell$ as sketched in Fig. 8(b). Then, we obtain the partially time-ordered integral

$$\begin{aligned}
& \int_{-\infty}^{\infty} ds_1 \int_{s_1}^{\infty} ds_2 \cdots \int_{s_{k-1}}^{\infty} ds_k \int_0^{\infty} d\tau_1 \cdots d\tau_k \\
& \times \exp \left[\frac{i}{\hbar} (\varepsilon_{a'} - \varepsilon_{a_{k-1}}) s_k + \frac{i}{\hbar} \sum_{\ell=2}^{k-1} (\varepsilon_{a_\ell} - \varepsilon_{a_{\ell-1}}) s_\ell \right. \\
& + \frac{i}{\hbar} (\varepsilon_{a_1} - \varepsilon_a) s_1 + \frac{i}{\hbar} \sum_{\ell=1}^k v_{b_\ell} \tau_\ell s_\ell \\
& \left. - \frac{i}{\hbar} \sum_{\ell=1}^k \left(\varepsilon_{b_\ell} - \varepsilon_{a'} - \frac{\tau_\ell}{2} - \sum_{\ell'=1}^{\ell-1} \tau_{\ell'} \right) \tau_\ell \right]. \quad (\text{A13})
\end{aligned}$$

Setting $a_k = a'$ and $a_0 = a$, one sees that all s integrals are of the form

$$\int_{-\infty}^{\infty} ds_\ell \exp[i(\varepsilon_{a_\ell} - \varepsilon_{a_{\ell-1}} + v_{b_\ell} \tau_\ell) s_\ell], \quad (\text{A14})$$

where the lower integration limit can be finite or $-\infty$. Evaluating this integral, one finds two types of terms: The first one is a principal value which is always regular and, thus, will not contribute to S_k . A second term is proportional to the delta function $\delta(\varepsilon_{a_\ell} - \varepsilon_{a_{\ell-1}} + v_{b_\ell} \tau_\ell)$. This will contribute if and only if its singularity is located at $\tau_\ell = 0$, as discussed above. Therefore, we find that energies of all participating a states must be identical,

$$\varepsilon_{a'} = \varepsilon_{a_1} = \cdots = \varepsilon_{a_k} = \varepsilon_a. \quad (\text{A15})$$

In the absence of degeneracies in the spectrum of the a states, the important condition follows that all nonvanishing contributions to the perturbation series must fulfill the relation

$$a' = a_1 = \cdots = a_k = a. \quad (\text{A16})$$

This selection rule states that the only allowed processes are those in which the system jumps repeatedly from the initial state to one of the b states and back. Note that this selection rule holds only for the contributions to the *final* transition probability at time $t = \infty$. At intermediate times, other a states can be populated as well, as has been exemplified in a numerical study of Landau-Zener transitions of a qubit coupled to a single harmonic oscillator.¹⁸

By use of the selection rule (A16), we obtain from (A13) for the $2k$ th-order term $\langle a | S_k | a \rangle$ the expression

$$\begin{aligned}
& \sum_{a_1 \cdots a_{k-1}} \sum_{b_1 \cdots b_k} |X_{ab_k}|^2 |X_{ab_{k-1}}|^2 \cdots |X_{ab_1}|^2 \\
& \times \int_{-\infty}^{\infty} ds_1 \int_{s_1}^{\infty} ds_2 \cdots \int_{s_{k-1}}^{\infty} ds_k \int_0^{\infty} d\tau_1 \cdots d\tau_k \\
& \times \exp \left(i \sum_{\ell=1}^k \frac{v_{b_\ell} \tau_\ell s_\ell}{\hbar} \right) \\
& \times \exp \left[- \frac{i}{\hbar} \sum_{\ell=1}^k \left(\varepsilon_{b_\ell} - \varepsilon_a - \frac{\tau_\ell}{2} - \sum_{\ell'=1}^{\ell-1} \tau_{\ell'} \right) \tau_\ell \right]. \quad (\text{A17})
\end{aligned}$$

A most important observation now is that the matrix elements X_{ab_ℓ} no longer depend on the index a_ℓ . Any permutation of the integration variables s_ℓ can therefore be undone by proper relabeling. Thus, we can replace the s integrals in the second line of (A17) by the symmetrized version

$$\frac{1}{k!} \int_{-\infty}^{\infty} ds_1 \cdots ds_k \exp \left(\frac{i}{\hbar} \sum_{\ell=1}^k v_{b_\ell} \tau_\ell s_\ell \right) = \frac{(2\pi\hbar)^k \delta(\tau_1) \cdots \delta(\tau_k)}{k! v_{b_1} \cdots v_{b_k}}. \quad (\text{A18})$$

The remaining τ integrations can be evaluated as well, each of which yielding $1/2$, so that finally

$$\langle a | S_k | a \rangle = \frac{1}{k!} \left(\pi\hbar \sum_b \frac{|X_{ab}|^2}{v_b} \right)^k. \quad (\text{A19})$$

Inserting this into the series (A5), we obtain the exact nonadiabatic Landau-Zener transition probability

$$P_{a \rightarrow a} = \exp \left(- \frac{2\pi}{\hbar} \sum_b \frac{|\langle a | X | b \rangle|^2}{v_b} \right), \quad (\text{A20})$$

where $X = \sum_{a,b} |a\rangle X_{ab} \langle b| + \text{H.c.}$ denotes the off-diagonal part of the Hamiltonian (A1). This formula generalizes our previous results.^{18,38} Similar formal results, though not applied to quantum dissipation, have been presented in the very recent work by Volkov and Ostrovsky.⁷⁵

Of much practical importance is the case in which all b states have the same velocity, $v_b = v$, so that we face a situation of two crossing energy bands. Owing to $\langle a | X | a' \rangle = 0$ for all a, a' , one finds $\sum_b \langle a | X | b \rangle \langle b | X | a \rangle = \langle a | X^2 | a \rangle$. For a nondegenerate initial state $|a\rangle$, we end up with^{18,38}

$$P_{a \rightarrow a} = \exp \left(- \frac{2\pi \langle a | X^2 | a \rangle}{\hbar v} \right). \quad (\text{A21})$$

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