Quantum dynamics of a two-state system in a dissipative environment

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An analytical study of the dissipative Landau-Zener model is presented. The model where two energy levels at constant speed are brought to cross is a standard model used to describe a large variety of phenomena. In many cases of interest the presence of coupling of the two-state system to an environment is of importance, the accounting for which shall be done here from first principles. Analytical results for the excitation transition from the ground state of the two-state system at large negative times to the excited state at large positive times (as well as the opposite, decay, transition) are obtained in terms of the speed by which the two levels approach each other, the energy gap between the adiabatic energies, the coupling strength to the environment, and its temperature. For the excitation transition we find the following results: In the slow-passage limit of small sweeping speed it is shown that adiabaticity is limited to low temperatures and the quantitative adiabatic criterion is established. Particularly, at zero temperature there is no influence of the environment on the transition probability as a consequence of a compensation property shown to be peculiar to the linear-sweep model. The transition is at low temperatures due to quantum tunneling and, with an increase in temperature, an intermediate region appears where the transition is dominated by thermally assisted transitions across the energy gap before finally at high temperatures a saturated regime is reached with equal population of the levels. In contrast to the dependence on the temperature the dependence of the transition probability as a function of coupling strength is nonmonotonic with maximum influence at intermediate strength. In the fast-passage limit with rapid sweep speed there is no influence of the environment on the transition probability. For the decay transition the adiabatic limit does not exist for the linear-sweep model for physically relevant spectra of the environment and the decay transition is dominated by spontaneous emission, except in the fast-passage limit and the high-temperature limit where the decay transition probability equals the excitation probability.

I. INTRODUCTION

In a recent Letter[1] we presented the results of an analytical study of the influence of an environment on the quantum dynamics of a two-state system. In particular, we considered the Landau-Zener transition; that is, the explicitly time-dependent situation in which the energy levels of a quantum-mechanical system in the course of time by external means are brought close together, so that transitions between the levels take place. The transition takes place in the presence of an environment and we shall give a detailed account of the effects of such a dissipative environment. We consider a model which in the absence of coupling to an environment is the standard model used to describe a large variety of problems and show that, even in the presence of coupling to an environment, an extensive analytical treatment can be given.

The level crossing problem appears in numerous contexts not only in physics, but also in chemistry, through its relevance for chemical reaction kinetics,[2] as well as in biophysics.[3] In physics, the problem is encountered widely, from the solar-neutrino puzzle[4] to numerous situations in atomic and solid-state physics: Nuclear magnetic resonance,[5] aspects of the behavior of laser-irradiated atoms,[6] atomic collisions,[7] atoms scattering off surfaces,[8] and dielectric breakdown in solids[9] are all well-known examples. The question of the effect of dissipation on level crossing transitions, however, has also gained renewed interest in view of its relevance to mesoscopic systems, for example, for estimating the effect of Zener tunneling on the magnitude of diamagnetic currents in mesoscopic rings.[10] The level crossing transition in the presence of coupling to the many degrees of freedom of an environment, which has hardly received attention from a first-principles point of view, thus constitutes an important example of quantum dynamics in a dissipative environment and is the subject matter of the present paper.

The question of the effect of dissipation on the quantum-mechanical behavior of a macroscopic variable has received much recent interest in the context of macroscopic quantum tunneling and coherence[11] and with regard to the latter, the present paper addresses questions relevant for the possible observability of Bloch oscillations in Josephson junctions insofar as this effect can be considered the counterpart of the Bloch oscillations of an electron moving in a crystal under the influence of an external field. With respect to tunneling, the problem we shall consider corresponds to the macroscopic tunneling of the trapped flux in a superconducting quantum interference device (SQUID) for the situation where the external flux is being changed in the course of time.

A characteristic feature for the above physical phenomena is, for the case of a macroscopic degree of freedom, invariably, that for many situations of interest the fact that the degree of freedom of interest is coupled to an environment is of importance and one has to account for this circumstance in terms of its effect on the quantum dynamics. The purpose of the present paper is to report in detail on the results obtained for the dissipative Landau-Zener model. The main body of Ref. 1 was devoted to a discussion of the transition from the ground state to the excited state in the adiabatic limit since the obtained results corrected erroneous ones in the literature. In the present paper we shall present the full calculations for all possible expansion limits. Furthermore, we shall present the equivalent results for the other possible transition, the decay transition. We shall qualify the statement made in Ref. 1 on the identification of the strong-coupling limit with the high-temperature limit. In fact, in Ref. 1, we only quoted the high-temperature result and never stated the strong-coupling result explicitly. We shall, in addition, give a full account of the applied real-time Schwinger-Keldysh method. The method we employ is a general one and an example of the usefulness of the application of the methods of quantum field theory to problems in nonequilibrium quantum statistical mechanics. The formulation we have chosen applies to arbitrary nonequilibrium states and will be useful in further studies of dissipative quantum dynamics.

In outline, the paper is organized as follows: In Sec. II we introduce the Landau-Zener model for the case where an environment is present, and describe the problem to be investigated: The influence of dissipation on the transition from the ground state to the excited state, or equivalently, investigate how the presence of an environment destroys phase coherence. In Sec. III we study the slow-passage limit where the energy levels are slowly brought together and investigate the question of adiabaticity. In Sec. IV we deal with the strong-coupling limit and in Sec. V with the high-temperature limit. In Sec. VI we present the perturbative treatment of the coupling to the environment in the slow-passage limit, and in Sec. VII we deal with the fast-passage limit. In Sec. VIII we consider the influence of dissipation on the decay of the excited state. In Sec. IX we apply the obtained results to a discussion of physical situations of interest and in Sec. X we summarize and conclude. The Appendix contains a detailed description of the Schwinger-Keldysh technique adapted to the present problem.

II. THE LANDAU-ZENER TRANSITION IN A DISSIPATIVE ENVIRONMENT

In the absence of coupling to the environment, the nonadiabiatic transition problem we shall consider is customarily referred to as the Landau-Zener problem. Quantitatively, this level crossing problem is described in terms of a two-dimensional spinor problem, as given by the time-dependent system Hamiltonian $H_s(t)$

$$H_s(t)=vt\sigma_z+\Delta\sigma_x \ , \tag{2.1}$$

where σ_z and σ_x are Pauli matrices. Evidently, the Hamiltonian in Eq. (2.1) need not represent a physical spin in a time-dependent external magnetic field, although this, of course, is the case for the nuclear magnetic resonance situation mentioned in the Introduction, but refers, in general, to the situation in which only two levels need consideration. The first term represents the crossing energy levels and the second term the level repulsion. As we shall take advantage of in Sec. VI, the above Hamiltonian is an exactly solvable one.

For the description of the environment, we take a set of harmonic oscillators as represented by the bath Hamiltonian H_B,

$$H_B=\sum_\alpha \hbar\omega_\alpha(a_\alpha^\dagger a_\alpha+\tfrac{1}{2}) \ , \tag{2.2}$$

and for the interaction between system and environment, we take the coupling linear in the bath coordinate operator X,[12]

$$H_i=\sigma_z X \ , \tag{2.3}$$

$$X=\sum_\alpha \lambda_\alpha(a_\alpha^\dagger+a_\alpha) \ . \tag{2.4}$$

Here $a_\alpha^\dagger$ and a_α denote the boson creation and annihilation operators corresponding to the frequency ω_α and λ_α is the oscillator coupling constant.[13]

Our total Hamiltonian $H(t)$ is thus the spin-boson Hamiltonian with a time-dependent bias

$$H(t)=H_s(t)+H_B+H_i \ . \tag{2.5}$$

The model is specified by the energy gap 2Δ between the adiabatic levels and the effective coupling to the environment as described by the spectral function

$$J(\omega)=\frac{4}{\hbar^2}\sum_\alpha \lambda_\alpha^2\delta(\omega-\omega_\alpha) \tag{2.6}$$

and, as external parameters, we have the sweeping rate v (assumed positive in the following) describing the rate of change in energy due to the action of an external force, as well as the temperature T, since our calculational scheme allows evaluation of the transition probability at arbitrary temperatures.

The results we shall obtain are valid for any physical spectral function, but when definite expressions are desirable, we shall assume the typical form

$$J(\omega)=\eta\omega(\omega/\omega_c)^{s-1}\exp(-\omega/\omega_c) \ , \tag{2.7}$$

where η is the effective dimensionless coupling constant and ω_c the upper cutoff for the bath modes.

For the physical problems mentioned in the Introduction, the chosen model represents, to a varying degree of quantitative reliability, the relevant physics for the situation of interest. Furthermore, the model shall be shown to display a rich variety with regard to the question of destruction of phase coherence, and, in view of the complexity of the dynamical situation, the model is therefore of interest in itself since extensive analytical results can be obtained. Despite the widespread use of the model in the absence of the environment, a first-principles calculation including the effects of the environment has, to our knowledge, been attempted only in the adiabatic limit in Ref. 14 which arrives at conclusions contrary to the ones reached here. Results for the fast-passage limit have recently been considered[15] but we shall establish them in more generality. Certain aspects of the problem have previously been studied from a phenomenological point of view.[6,8,16] From our microscopic treatment we shall be able to assess the limits of validity of the results obtained by the phenomenological approaches. Furthermore, we shall point out a subtle compensation property of the model that has been missed by previous treatments.

Having established the model to be investigated, as represented by the above Hamiltonian, we can now pose the problem to be solved: At a remote time (which we for all purposes can take to be at time $t_0 = -\infty$), we assume that our initial state is described by some initial statistical operator ρ_i for which the system, that is, the spin, is in the ground state and we then ask for the probability P that the system in the far future is in its excited state while the bath is assumed unobserved. In Sec. VIII we shall study the other possible transition where the spin is initially in the excited state.

Various choices for the initial correlation between the spin and the environment can be taken. The bath could, for example, be assumed initially to be relaxed to the fixed initial spin direction or the other extreme, the two systems being initially decoupled with the bath assumed in thermal equilibrium. As expected, we can show that the results for the transition probability is the same for both these choices and therefore insensitive to the initial condition. For definiteness we shall henceforth choose the decoupled initial condition

$$\rho_i = |\uparrow\rangle\langle\uparrow|\rho_B = P_\uparrow \rho_B \tag{2.8}$$

such that ρ_B is the equilibrium statistical operator for the bath

$$\rho_B = \frac{\exp(-\beta H_B)}{\mathrm{tr}[\exp(-\beta H_B)]} , \tag{2.9}$$

where β is inversely proportional to the temperature T, $\beta^{-1} = k_B T$, and tr denotes trace over the environmental degrees of freedom.

We can now state the problem quantitatively: In terms of the evolution operator $U(t,t')$, corresponding to the total Hamiltonian $H(t)$ (below T denotes time ordering, but no confusion with temperature should arise)

$$U(t,t') = T \exp\left[-\frac{i}{\hbar}\int_{t'}^{t} d\bar{t}\, H(\bar{t}) \right] , \tag{2.10}$$

the transition or tunneling probability P for excitation is given by

$$P = \mathrm{Tr}[\rho_i U^\dagger(\infty,-\infty) P_\uparrow U(\infty,-\infty)] . \tag{2.11}$$

Here $P_\uparrow$ projects onto the spin-up state, $|\uparrow\rangle$, $\dagger$ denotes Hermitian conjugation, and Tr denotes the trace over all the degrees of freedom.

We shall now perform an analytic calculation of the transition probability and to this end employ the real-time quantum dynamical technique originally due to Schwinger and Keldysh[17] as this method allows calculations for externally driven systems at finite temperatures. The technical aspects of the method and the physical interpretation of the influence of an environment on the quantum dynamics of a single degree of freedom is given in the Appendix.

III. THE SLOW-PASSAGE LIMIT

In this section we shall calculate the transition probability in the slow-passage limit where the degree of freedom traverses the transition region slowly; that is, the Landau-Zener time $\tau_{LZ} = \Delta/v$ is much larger than the oscillation time of the two-level system $2\hbar/\Delta$ or, in terms of the dimensionless parameter $\gamma = \Delta^2/2\hbar v$, the limit where γ is larger than one. In the slow passage limit we expect an adiabatic evolution to take place and to facilitate the calculation, it is convenient to view the transition from the "adiabatic frame" by rotating around the y axis in spin space through the angle

$$\chi(t) = \mathrm{arccot}(-vt/\Delta) . \tag{3.1}$$

The corresponding time-dependent rotation operator is

$$R(t) = \exp\left[\frac{i}{2}\chi(t)\sigma_y \right] , \tag{3.2}$$

where the Pauli matrix σ_y is the generator of rotations around the y axis in spin space.

Performing this time-dependent unitary transformation, we obtain for the Hamiltonian in the adiabatic frame

$$\mathcal{H}(t) = H_0(t) + H_1(t) \tag{3.3}$$

with the adiabatic diagonal part

$$H_0(t) = -\varepsilon_t \sigma_z + \alpha_t \sigma_z X + H_B \tag{3.4}$$

and a transition-causing part

$$H_1(t) = \frac{\hbar v \Delta}{2\varepsilon_t^2}\sigma_y + \frac{\Delta}{\varepsilon_t}\sigma_x X . \tag{3.5}$$

Here we have introduced the adiabatic energy

$$\varepsilon_t = [(vt)^2 + \Delta^2]^{1/2}$$

and the abbreviated notation $\alpha_t = -vt/\varepsilon_t$ for the time-dependent coupling function to σ_z in the adiabatic frame. The time dependence of the crossing energy levels and the instantaneous eigenvalues for the system Hamiltonian are depicted in Fig. 1.

The first term in $H_1(t)$ describes the environment in-

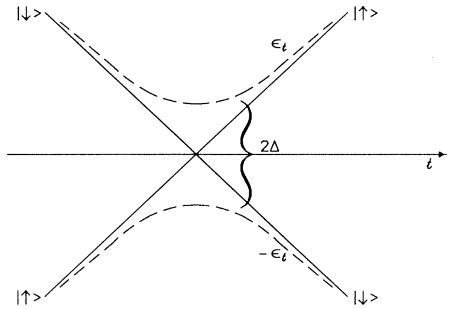

FIG. 1. The solid lines represent the crossing energy levels and the dashed lines the adiabatic energy levels.

dependent correction to adiabaticity as reflected by the transformation to the adiabatic frame being time dependent. The environment coupling to σ_z in Eq. (3.4) is now time dependent and weaker in the transition region as compared to the original frame, but in this region we now get an additional coupling to σ_x represented by the second term in $H_1(t)$, which causes transitions between the up- and down-spin states accompanied by phonon emissions and absorptions.

The evolution operator in the adiabatic frame $\tilde{U}$ corresponding to the Hamiltonian $\mathcal{H}(t)$

$$\tilde{U}(t,t')=T\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,\mathcal{H}(\bar{t})\right] \tag{3.6}$$

is related to the U of Eq. (2.10) by

$$U(t,t')=R(t)\tilde{U}(t,t')R^{\dagger}(t') \tag{3.7}$$

and the transition probability P is consequently given by the expression

$$P=\mathrm{Tr}[\rho_i\tilde{U}^{\dagger}(\infty,-\infty)P_{\downarrow}\tilde{U}(\infty,-\infty)] , \tag{3.8}$$

where $P_{\downarrow}$ projects onto the spin-down state $|\downarrow\rangle$.

We have partitioned in Eq. (3.3) the Hamiltonian $H(t)$ into diagonal and off-diagonal parts with respect to the z-direction in spin space in the adiabatic frame in order to be able to set up the perturbative expression in the off-diagonal nonadiabatic transition-causing part $H_1(t)$. Finally, we therefore switch to the interaction picture with respect to $H_0(t)$ and obtain the transition probability

$$P=\mathrm{Tr}[\rho_i V^{\dagger}(\infty,-\infty)P_{\downarrow}V(\infty,-\infty)] \tag{3.9}$$

in terms of the transition-causing evolution operator V given by

$$V(t,t')=T\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,H_1^I(\bar{t})\right] , \tag{3.10}$$

where

$$H_1^I(t)=U_0^{\dagger}(t,t_0)H_1(t)U_0(t,t_0) \tag{3.11}$$

and the evolution operator corresponding to $H_0(t)$ is

$$U_0(t,t')=T\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,H_0(\bar{t})\right] . \tag{3.12}$$

So far all is quite general and we have arrived at a formula, Eq. (3.9), that is convenient as starting point for a calculation in the adiabatic limit since it is sufficient to consider ony one flip of the spin.

Thus, by expanding V we get the expression for P in the adiabatic limit

$$P=\frac{1}{\hbar^2}\mathrm{tr}\left[\rho_B\left\langle\uparrow\left|\int_{-\infty}^{\infty}dt\,H_1^I(t)\right|\downarrow\right\rangle\times\left\langle\downarrow\left|\int_{-\infty}^{\infty}dt'H_1^I(t')\right|\uparrow\right\rangle\right] . \tag{3.13}$$

We can now get rid of the explicit appearance of the spin operators by utilizing the fact that $H_0(t)$ is diagonal in space space and rewrite Eq. (3.13) as

$$P=\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2 I(t_1,t_2)\times\exp\{i[\phi_0(t_2)-\phi_0(t_1)]\} , \tag{3.14}$$

where I describes the flip of the spin

$$I(t_1,t_2)=\langle U_1^{\dagger}(t_1,t_0)B[\varepsilon_{t_1},X(t_1)]U_{-1}(t_1,t_2)\times B^{\dagger}[\varepsilon_{t_2},X(t_2)]U_1(t_2,t_0)\rangle \tag{3.15}$$

and ϕ_0 is the bare phase

$$\phi_0(t)=\frac{2}{\hbar}\int_{-\infty}^{t}dt'\varepsilon_{t'} . \tag{3.16}$$

We have introduced the shorthand notation for the act of the flip

$$B[\varepsilon_t,X(t)]=\frac{\Delta v}{2\varepsilon_t^2}+i\frac{\Delta}{\hbar\varepsilon_t}X(t) \tag{3.17}$$

and the adiabatic evolution gives rise to the factors

$$U_{\pm 1}(t,t')=T\exp\left[(\pm 1)\frac{-i}{\hbar}\int_{t'}^{t}d\bar{t}\,\alpha_{\bar{t}}X(\bar{t})\right] , \tag{3.18}$$

where the bath operator in the interaction picture is given by

$$X(t)=\exp\left[\frac{i}{\hbar}H_B t\right]X\exp\left[-\frac{i}{\hbar}H_B t\right] . \tag{3.19}$$

The brackets $\langle\cdots\rangle$ in Eq. (3.15) denote $\mathrm{tr}(\rho_B\cdots)$.

The fact that the probability is a real number is, at this point, represented by the following Hermitian property of the integrand I of Eq. (3.14):

$$I(t_1,t_2)=I^*(t_2,t_1) , \tag{3.20}$$

where $*$ denotes a complex conjugation.

This property allows us to choose a definite time-ordering relation between t_1 and t_2 so that Eq. (3.14) can be rewritten in its explicit real form

$$P=2\,\mathrm{Re}\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{t_1}dt_2 I(t_1,t_2)\times\exp\{i[\phi_0(t_2)-\phi_0(t_1)]\}\ . \quad (3.21)$$

We shall now employ the real-time dynamical technique as it is convenient to relate the term in the brackets of Eq. (3.15) to an expression involving the closed-time-path Green's function for the bath.[18] In order to do so, we introduce the generating functional for the environmental coordinate along the closed time path c, extending back and forth along the real axis[17,18]

$$Z[\zeta]=\left\langle T_c\exp\left[-\frac{i}{\hbar}\int_c d\tau\,\zeta(\tau)X(\tau)\right]\right\rangle\ , \quad (3.22)$$

where T_c denotes the contour-ordering operator along the closed contour c, extending from $-\infty$ to $+\infty$ and back again to $-\infty$. Employing functional differentiation, we can then express Eq. (3.21) as

$$P=2\,\mathrm{Re}\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{t_1}dt_2\exp\{i[\phi_0(t_2)-\phi_0(t_1)]\}\times B\left[\varepsilon_{t_1},i\hbar\frac{\delta}{\delta\zeta_1(t_1)}\right]\times B^\dagger\left[\varepsilon_{t_2},i\hbar\frac{\delta}{\delta\zeta_1(t_2)}\right]Z[\zeta]|_{\zeta=\zeta^0} \quad (3.23)$$

provided we, after the functional differentiation, insert the proper "force" $\zeta=\zeta^0$. On the forward contour from $-\infty$ to $+\infty$, we shall choose

$$\zeta(t)=\zeta_1^0(t)=\alpha_t\{1-2[\Theta(t-t_2)-\Theta(t-t_1)]\}=\begin{cases}\alpha_t, & -\infty<t<t_2\ ,\\ -\alpha_t, & t_2<t<t_1\ ,\\ \alpha_t, & t_1<t<\infty\ ,\end{cases} \quad (3.24)$$

where Θ denotes the step function, and on the backward contour from $+\infty$ to $-\infty$, we shall choose

$$\zeta(t)=\zeta_2^0(t)=\alpha_t,\quad -\infty<t<\infty\ . \quad (3.25)$$

We note the characteristic of dissipative dynamics that the "force" ξ^0 is different on the forward and backward time paths, in contrast to an external classical force.

The calculation of the probability P has now been reduced to the calculation of the generating functional Z, which for the present case of a set of harmonic oscillators is easily done according to Wick's theorem[19]

$$Z[\zeta]=\exp\left[-\frac{i}{2\hbar^2}\int_c d\tau\int_c d\tau'\zeta(\tau)D(\tau,\tau')\zeta(\tau')\right]\ , \quad (3.26)$$

where we have introduced the contour-ordered Green's function along the closed time patch c for the bath

$$D(\tau,\tau')=-i\langle T_c[X(\tau)X(\tau')]\rangle\ . \quad (3.27)$$

We can now evaluate P and obtain for the probability, after taking advantage of the interrelationships between the Green's functions appearing when τ and τ' resides on the forward or backward part of the contour[20] (for details we refer to the Appendix),

$$P=2\,\mathrm{Re}\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{t_1}dt_2\left[a^*(t_2,t_1)a(t_1,t_2)+\left[\frac{\Delta}{\hbar}\right]^2\frac{i}{\varepsilon_{t_1}\varepsilon_{t_2}}D_{11}(t_1,t_2)\right]Z(t_1,t_2)\exp\{i[\phi_0(t_2)-\phi_0(t_1)]\}\ , \quad (3.28)$$

where

$$a(t_1,t_2)=\frac{v\Delta}{2\varepsilon_{t_1}^2}+i\frac{\Delta}{\hbar^2\varepsilon_{t_1}}\left[\int_{-\infty}^{\infty}dt\,D^R(t_1,t)\alpha_t-2\int_{t_2}^{t_1}dt\,D_{11}(t_1,t)\alpha_t\right] \quad (3.29)$$

and, upon inserting $\zeta=\zeta_0$, $Z[\zeta]$ becomes the function of t_1 and t_2 (when $t_1>t_2$; for the opposite sequence we have the complex conjugate)

$$Z(t_1,t_2)=\exp\left[-\frac{i}{\hbar^2}\int_{t_2}^{t_1}dt\int_{t_2}^{t_1}dt'\alpha_t D^K(t,t')\alpha_{t'}\right]\exp\left[\frac{2i}{\hbar^2}\int_{t_2}^{t_1}dt\int_{-\infty}^{t_2}dt'\alpha_t D^R(t,t')\alpha_{t'}\right]\ . \quad (3.30)$$

The Green's functions introduced are the retarded, Keldysh, and usual time ordered:[20]

$$D^R(t,t')=-i\Theta(t-t')\langle[X(t),X(t')]\rangle=-\frac{\hbar^2}{2}\Theta(t-t')\int_0^{\infty}d\omega\,J(\omega)\sin\omega(t-t')\ , \quad (3.31)$$

$$D^K(t,t')=-i\langle\{X(t),X(t')\}\rangle=-\frac{i}{2}\hbar^2\int_0^{\infty}d\omega\,J(\omega)\coth(\hbar\omega/2k_BT)\times\cos\omega(t-t')\ , \quad (3.32)$$

$$D_{11}(t,t')=-i\langle T[X(t)X(t')]\rangle=\tfrac{1}{2}[D^R(t,t')+D^R(t',t)+D^K(t,t')]\ . \quad (3.33)$$

We have now achieved the goal of getting rid of operators and expressed the transition probability in terms of integrals. In the following we shall show that, under certain conditions which establish the adiabatic limit, we can, in fact, perform the time integrals and obtain a closed expression for the transition probability in terms of known functions.

We note that the expression Eq. (3.28) for the probability can be written in the more suggestive form using the hermiticity property Eq. (3.20)

$$P=\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2\,A(t_1,t_2)\exp[i\tilde{\phi}(t_1,t_2)]\ . \tag{3.34}$$

Here the phase factor contains, in addition to the bare phase ϕ_0, a contribution ϕ due to the influence of the interaction

$$\tilde{\phi}(t_1,t_2)=\phi_0(t_2)-\phi_0(t_1)+\phi(t_1,t_2)\ , \tag{3.35}$$

where

$$\phi(t_1,t_2)=-\int_{-\infty}^{t_1}dt\int_{-\infty}^{t_2}dt'\int_0^{\infty}d\omega\,J(\omega)\alpha_t\times\sin[\omega(t-t')]\alpha_{t'}\ . \tag{3.36}$$

The "amplitude" factor is given by

$$A(t_1,t_2)=\left[\frac{v\Delta}{2\varepsilon_{t_1}\varepsilon_{t_2}}\right]^2\tilde{A}(t_1,t_2) \tag{3.37}$$

and $\tilde{A}$ is the function

$$\tilde{A}(t_1,t_2)=\hat{A}(t_1,t_2)|Z(t_1,t_2)|\ , \tag{3.38}$$

where

$$\hat{A}(t_1,t_2)=\left[\frac{2\varepsilon_{t_1}\varepsilon_{t_2}}{v\Delta}\right]^2\left[a^*(t_2,t_1)a(t_1,t_2)+\left[\frac{\Delta}{\hbar}\right]^2\frac{i}{\varepsilon_{t_1}\varepsilon_{t_2}}D^>(t_1,t_2)\right] \tag{3.39}$$

and the absolute value of Z does not depend on the retarded bath Green's function

$$|Z(t_1,t_2)|=\exp\left[\frac{-i}{\hbar^2}\int_{t_2}^{t_1}dt\int_{t_2}^{t_1}dt'\alpha_t D^K(t,t')\alpha_{t'}\right]\ . \tag{3.40}$$

The introduced correlation function is

$$D^>(t,t')=-i\langle X(t)X(t')\rangle=\tfrac{1}{2}[D^R(t,t')-D^R(t',t)+D^K(t,t')]\ . \tag{3.41}$$

Except for the factor $\hat{A}$, the "amplitude" factor is a real positive function. However, in the evaluation of the transition probability in the stationary phase approximation performed below, the effect of the function $\hat{A}$ reduces to a multiplicative factor which by the chosen normalization equals one.

The integrals in Eq. (3.34) in the expression for P can be evaluated by employing a stationary phase method since the free phase ϕ_0 provides a fast oscillating phase factor provided that the "adiabatic" parameter γ is large, $\gamma>1$. In the absence of coupling to the environment, the integrals over t_1 and t_2 are uncoupled and dominated by the stationary phase point of ϕ_0 which, for the integral over t_1, must be chosen as $i\tau_{LZ}$ and for t_2 the complex conjugate number $-i\tau_{LZ}$. As we shall demonstrate shortly, if $\eta<\gamma\omega_c\tau_{LZ}$, then this is also the case in the presence of the environment. We therefore deform the integration contour into the complex time plane as shown in Fig. 2. Our choice of contour must avoid the stationary point of ϕ_0 since the prefactor A is singular at this point, which, furthermore, is the end point of the integrand's branch cut as depicted in Fig. 2. We note that, calculating the probability in the absence of coupling by the stationary phase method, we obtain the exact result [see Eq. (6.37)] up to a small logarithmic correction

$$\tilde{P}_0=(\pi/4)^2\exp(-2\pi\gamma)\ . \tag{3.42}$$

Away from the stationary phase point of ϕ_0, $|\mathrm{Re}t|>\tau_{LZ}$, ϕ_0 is a rapidly oscillating function since it is proportional to γ and we therefore need to keep only the contributions from the small semicircle parts of the integration contours. The rest of the integrand

$$\tilde{A}(t_1,t_2)\exp[i\phi(t_1,t_2)]$$

is, as long as the temperature T satisfies $k_BT\le\Delta/4\gamma$, a smooth function of t_1 and t_2. Thus, we can quantity the adiabatic limit to mean $\gamma>1$ as well as $k_BT\le\Delta/4\gamma$, and in this limit we have, for the transition probability P,

$$P=\tilde{A}(i\tau_{LZ},-i\tau_{LZ})\exp[i\phi(i\tau_{LZ},-i\tau_{LZ})]\tilde{P}_0\ . \tag{3.43}$$

This expression, as noted above, reduces to

$$P=Z(i\tau_{LZ},-i\tau_{LZ})\tilde{P}_0\ . \tag{3.44}$$

We are thus left with calculating the quantity $Z(i\tau_{LZ},-i\tau_{LZ})$. At this point, it is not evident that we can express the result in closed form, but in the linear sweep model under consideration the integrals appearing can be expressed in terms of known functions. In fact, after noticing the cancellation between a term in $|Z(i\tau_{LZ},-i\tau_{LZ})|$ and the term

$$\exp[i\phi(i\tau_{LZ},-i\tau_{LZ})]$$

we obtain an expression for the tunneling probability P in the adiabatic limit, valid for $\gamma>1$ and $k_BT\le\Delta/4\gamma$, which can be expressed in closed form

$$P=\tilde{P}_0\exp[\mathcal{E}(T,\tau_{LZ})] \tag{3.45}$$

with the environment-dependent exponent $\mathcal{E}$ given by

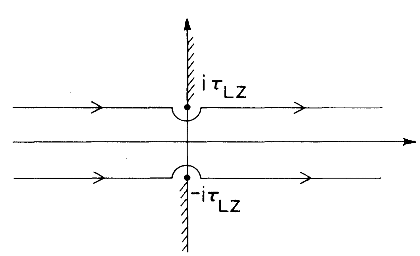

FIG. 2. Adiabatic integration contours in the complex-time plane with branch cuts indicated.

$$\mathscr{E}(T,\tau_{\rm LZ})=\ln Z(i\tau_{\rm LZ},-i\tau_{\rm LZ})$$
$$=\pi^2\tau_{\rm LZ}^2\int_0^\infty d\omega\, J(\omega)n(\omega)I_1^2(\omega\tau_{\rm LZ}) , \quad (3.46)$$

where n is the Bose function and I_1 is the modified Bessel function. The temperature dependence originally appears only in $|Z|$ and there in form of a thermal and quantum fluctuation (zero-point) term

$$\coth(\hbar\omega/2k_BT)=2n(\omega)+1 .$$

The above-mentioned cancellation is the exact cancellation of the systematic, dissipative term

$$\exp[i\phi(i\tau_{\rm LZ},-i\tau_{\rm LZ})]$$

by the quantum fluctuations or quantum noise term. The quantum noise term alone leads to an increase in the transition probability at zero temperature; this is due to the circumstance that the exponentially small bare transition probability is a result of a delicate destructive interference between amplitudes which, in the presence of the quantum noise, is partially upset. The canceling systematic force term effectively renormalizes the adiabatic parameter γ, and constitutes a combined renormalization of the energy gap and the sweeping rate. For the general distinction between the two terms and their relationship through the fluctuation-dissipation theorem, we refer to the general discussion in the Appendix. Surprisingly, we thus find that, in the adiabatic limit at zero temperature, the transition probability is not affected by the presence of the coupling to the environment as $\mathscr{E}(T=0,\tau_{\rm LZ})$ is equal to zero.

The exact compensation leading to the absence of influence of the environment at zero temperature is a property of the considered model; to be specific, the linear form of the external drive $vt\sigma_z$. We have also studied models where the external drive is not linear in time and there we find only partial cancellation. The canceling systematic term is minimal for the linear-sweep model and for other cases we thus find that the zero-temperature transition probability is decreased by the presence of the coupling to the environment.

As noted earlier, in order for adiabaticity to prevail, we must require that the temperature T is smaller than $\Delta/4\gamma k_B$. If this requirement is not satisfied, terms involving D^K will be ultraviolet divergent and our assumption of Z being a smoothly varying function, necessary for the stationary phase method to be applicable, ceases to be valid; or, in other words, the bare stationary phase point determined by the bare phase ϕ_0 is no longer a good approximation to the true stationary phase point. The breakdown of adiabaticity at low (on the scale of Δ/k_B) temperatures is a consequence of thermal activation which destroys adiabaticity. Lastly, we must argue that maintaining only the lowest-order term in H_1^I in Eq. (3.9) for the transition probability P does not amount to a perturbative treatment of the coupling; in fact, in the strong-coupling limit, adiabaticity is recovered, as we shall show in the next section. This is readily done as long as the integrals are controlled by the bare stationary phase point, since then such terms, like $\hat{A}$ of Eq. (3.39), has a prefactor which is small near the bare stationary phase point. The crucial question for the validity of our calculation in the adiabatic limit is therefore the extent to which the bare stationary phase points are sufficient. One restriction for this to be valid we have mentioned already, namely, that the temperature has to be sufficiently low, $k_BT\leq\Delta/4\gamma$; another question is the restriction this implies for the coupling strength. We have, to this end, investigated the position of the exact stationary phase point as a function of the coupling strength and find that the position of the stationary phase point, after initially moving further out in the complex plane for sufficiently strong coupling, moves to the real axis (in fact, very close to origin, $t_s=\pi/\omega_c$, in which case our calculational scheme has long ceased to be valid). However, this happens only when the coupling strength η is of order $\gamma\omega_c\tau_{\rm LZ}$. Since this criterion only excludes extremely strong coupling, we find that the stationary phase calculation is not restricted to weak coupling.

The result Eqs. (3.45) and (3.46) differs qualitatively as well as quantitatively from the, to our knowledge, only other published result in the literature[14] on the influence of dissipation in this model in the adiabatic limit. Firstly, at zero temperature we do not find any depression of the tunneling probability as in Ref. 14, the reason being the compensation between the renormalization and quantum noise effects. Secondly, our result is not plagued by infrared divergences for any physical choice of the spectral function. The above result leads to the opposite conclusion, in general, as compared to the result of Ref. 14. The difference is due to the use of their Eq. (2.28) for the adiabatic energy difference in the phase factor which is insufficient as it neglects the equally important coupling contribution to the adiabatic energy.

The slow-passage, low-temperature result lends itself to a simple interpretation: At zero temperature the transition can take place only through quantum tunneling but with probability unmodified as compared to the uncoupled case. At finite temperatures, the transition probability is enhanced due to phonon-assisted transitions.

IV. THE STRONG-COUPLING LIMIT

In the preceding section we found that our scheme of calculating the transition probability in the slow-passage limit eventually would break down for strong enough coupling. A different question, which we now turn to, is whether adiabaticity is lost in the case of strong coupling.

In order to answer this question, we start out from the exact perturbation expression in the tunneling matrix element Δ for the transition probability P that emerges when one first eliminates the spin degree of freedom and subsequently performs the trace over the bath degrees of freedom. The expression can be obtained with equal ease from a path-integral approach[21] or by the real-time generating functional technique. For completeness and further elaboration of our formulation, we have demonstrated the latter method in detail in the Appendix where we obtain the result (we follow the notation of Leggett *et al.*[21])

$$P=1+\tfrac{1}{2}\sum_{n=1}^{\infty}(-1)^n\int_{-\infty}^{\infty}dt_{2n}\int_{-\infty}^{t_{2n}}dt_{2n-1}\cdots\int_{-\infty}^{t_2}dt_1\widetilde{F}_n(t_1,t_2,\ldots,t_{2n})\,, \tag{4.1}$$

where the integrand

$$\widetilde{F}_n=\left[\frac{2\Delta}{\hbar}\right]^{2n}2^{-n}\sum_{(\zeta_j=\pm 1)}^{\infty}F_1F_2F_3F_4 \tag{4.2}$$

is given by ($F_{1\text{-}4}$ being functions of $t_1,\ldots,t_{2n}$ as well as of the ζ_j's)

$$F_1=\exp\left[-\sum_{j=1}^{n}S_j\right]\,, \tag{4.3}$$

$$F_2=\exp\left[\sum_{k=1}^{n}\sum_{j=k+1}^{n}\zeta_j\Lambda_{jk}\zeta_k\right]\,, \tag{4.4}$$

$$F_3=\prod_{k=2}^{n}\cos\left[\sum_{j=k+1}^{n}\zeta_jX_{jk}\right]\,, \tag{4.5}$$

$$F_4=\cos\left[\sum_{j=1}^{n}\zeta_j\left[\frac{v}{\hbar}(t_{2j}^2-t_{2j-1}^2)-X_{j0}\right]\right]\,, \tag{4.6}$$

$$S_j=Q_2(t_{2j}-t_{2j-1})\,, \tag{4.7}$$

$$\Lambda_{jk}=Q_2(t_{2j}-t_{2k-1})+Q_2(t_{2j-1}-t_{2k})-Q_2(t_{2j}-t_{2k})-Q_2(t_{2j-1}-t_{2k-1})\,, \tag{4.8}$$

$$X_{jk}=Q_1(t_{2j}-t_{2k+1})+Q_1(t_{2j-1}-t_{2k})-Q_1(t_{2j}-t_{2k})-Q_1(t_{2j-1}-t_{2k+1})\,, \tag{4.9}$$

$$Q_1(t)=\int_0^{\infty}d\omega\,\omega^{-2}J(\omega)\sin\omega t=\frac{1}{\hbar^2}\int_0^t d\overline{t}\int_0^t d\overline{t}'D^R(\overline{t},\overline{t}')+t\int_0^{\infty}d\omega\frac{J(\omega)}{\omega}\,, \tag{4.10}$$

$$Q_2(t)=\int_0^{\infty}d\omega\,\omega^{-2}J(\omega)(1-\cos\omega t)\coth(\tfrac{1}{2}\beta\hbar\omega)=\frac{i}{\hbar^2}\int_0^t d\overline{t}\int_0^t d\overline{t}'D^K(\overline{t},\overline{t}')\,. \tag{4.11}$$

In Eqs. (4.10) and (4.11), we have explicitly stated the relation between the function Q_1 and the retarded response function D^R for the bath, and the function Q_2 and the correlation function for the bath D^K. We postpone the interpretation of the functions to the next section.

The above general expression is too complicated to allow further progress; however, we shall argue that, in the strong-coupling limit, we can, in our driven and therefore time-dependent case, also apply the so-called noninteracting blip approximation.[22] This approximation is allowable because, crudely speaking, the coupling suppresses blips; that is, time intervals where the reduced density matrix of the spin is off diagonal ($\zeta_j=-1$) and extends, sojourns where the reduced density matrix is diagonal ($\zeta_j=1$), so that only nearest-neighboring blips interact. For a detailed discussion of the noninteracting blip approximation we refer to Leggett *et al.*[21] Explicitly, the noninteracting blip approximation amounts to setting all Λ_{jk} equal to zero as well as the X_{jk} with $k\neq j-1$, and approximate the rest of the X_{jk}'s by the first term in Eq. (4.9). The prescription for the noninteracting blip approximation is thus

$$\Lambda_{jk}=0 \tag{4.12}$$

and

$$X_{jk}=\delta_{j,k+1}Q_1(t_{2j}-t_{2j-1})\,. \tag{4.13}$$

The expression for $F_{2\text{-}4}$ then reduces to (F_1 is unchanged)

$$F_2=1\,, \tag{4.14}$$

$$F_3=\prod_{k=2}^{n}\cos[Q_1(t_{2k}-t_{2k-1})]\,, \tag{4.15}$$

$$F_4=\cos\left[\sum_{k=1}^{n}\zeta_k\frac{v}{\hbar}(t_{2k}^2-t_{2k-1}^2)\right]\times\cos[\zeta_1Q_1(t_2-t_1)]+\sin\left[\sum_{k=1}^{n}\zeta_k\frac{v}{\hbar}(t_{2k}^2-t_{2k-1}^2)\right]\sin[\zeta_1Q_1(t_2-t_1)]\,. \tag{4.16}$$

The summation over the set $\{\zeta_j\}$ in Eq. (4.2) can now be carried out and we obtain, in the noninteracting blip approximation for $\widetilde{F}_n$, the result

$$\widetilde{F}_n=\left[\frac{2\Delta}{\hbar}\right]^{2n}\prod_{j=2}^{n}\exp[-Q_2(t_{2j}-t_{2j-1})]\cos[Q_1(t_{2j}-t_{2j-1})]\cos\left[\frac{v}{\hbar}(t_{2j}^2-t_{2j-1}^2)\right]$$
$$\times\exp[-Q_2(t_2-t_1)]\left[\cos\left[\frac{v}{\hbar}(t_2^2-t_1^2)\right]\cos[Q_1(t_2-t_1)]+\sin\left[\frac{v}{\hbar}(t_2^2-t_1^2)\right]\sin[Q_1(t_2-t_1)]\right] \tag{4.17}$$

and subsequently, for the transition probability,

$$P=1+\tfrac{1}{2}\sum_{n=1}^{\infty}(-1)^n\int_{-\infty}^{\infty}dt_{2n}\int_{-\infty}^{t_{2n}}dt_{2n-1}\cdots\int_{-\infty}^{t_2}dt_1\left[\prod_{j=1}^{n}g(t_{2j},t_{2j-1})+h(t_2,t_1)\prod_{j=2}^{n}g(t_{2j},t_{2j-1})\right]\,, \tag{4.18}$$

where the functions g and h are given by

$$g(t_2,t_1)=\left[\frac{2\Delta}{\hbar}\right]^2\cos\left[\frac{v}{\hbar}(t_2^2-t_1^2)\right]\times\cos[Q_1(t_2-t_1)]\exp[-Q_2(t_2-t_1)] \quad (4.19)$$

and

$$h(t_2,t_1)=\left[\frac{2\Delta}{\hbar}\right]^2\sin\left[\frac{v}{\hbar}(t_2^2-t_1^2)\right]\times\sin[Q_1(t_2-t_1)]\exp[-Q_2(t_2-t_1)] . \quad (4.20)$$

The integrand in Eq. (4.18) is still too complicated to allow for an exact evaluation of the integrals. However, the expression in Eq. (4.18) is considerably simpler than the exact expression of Eqs. (4.1)–(4.11) and can, in fact, as we shall demonstrate, in certain limits be evaluated. In order to simplify the expression in Eq. (4.18), we can take advantage of the fact that the function $Q_2(t)$ is small only for times $t\le(\eta\omega_c^2)^{-1/2}$. To demonstrate this let us note that, at zero temperature, we have[21]

$$Q_2(t)=\begin{cases}\eta\Gamma(s)(1-s)^{-1}[1-\mathrm{Re}(1+i\omega_c t)^{1-s}] , & 0<s<1 ,\\ \frac{1}{2}\eta\ln(1+\omega_c^2t^2), & s=1 ,\\ \eta\Gamma(s-1)[1-\mathrm{Re}(1-i\omega_c t)^{1-s}] , & s>1 ,\end{cases} \quad (4.21)$$

and (for arbitrary temperature)

$$Q_1(t)=\begin{cases}\eta\Gamma(s)(1-s)^{-1}\mathrm{Im}(1+i\omega_c t)^{1-s} , & 0<s<1 ,\\ \eta\tan^{-1}\omega_c t, & s=1 ,\\ \eta\Gamma(s-1)\mathrm{Im}(1-i\omega_c t)^{1-s}, & s>1 ,\end{cases} \quad (4.22)$$

where Γ denotes the gamma function.

For our subsequent approximation scheme to work, we need to observe that $Q_2(t)\le 1$ only for times $t\le(\eta\omega_c^2)^{-1/2}$. In fact, we then have, as long as $\omega_c t<1$ also, the following behavior:

$$Q_2(t)=\tfrac{1}{2}\Gamma(s)\eta\omega_c^2t^2 \quad (4.23)$$

and

$$Q_1(t)=\Gamma(s)\eta\omega_c t . \quad (4.24)$$

If we therefore require

$$\sqrt{\eta}>1 , \quad (4.25)$$

the dominating contribution in the strong-coupling limit to the expression Eq. (4.18) for the transition probability can be found. We shall call condition (4.25) the strong-coupling criterion, and note that, if it is satisfied, only small [compared to $(\eta\omega_c^{1+s})^{-1/2}$] time differences $|t_{2j}-t_{2j-1}|$ give a significant contribution to the integral in Eq. (4.18). The exponential suppression of the functions g and h by the factor containing Q_2 therefore limits the range of integration to time differences δ, where $\delta=(\eta\omega_c^2)^{-1/2}$. Introducing this time difference cutoff allows us to replace exponentials containing Q_2 by unity. Furthermore, the terms containing Q_1 are oscillatory functions with frequency $\Gamma(s)\eta\omega_c$ for times $t<\omega_c^{-1}$, and constants for larger times. In order to exploit this fact we perform the following change of variables:

$$x_k=\sum_{j=1}^{2k-1}(-1)^{j+1}t_j,\quad 1\le k\le n , \quad (4.26)$$

$$y_k=t_{2k}-t_{2k-1},\quad 1\le k\le n . \quad (4.27)$$

In the expression

$$t_{2j}^2-t_{2j-1}^2=2y_j\left[x_j-\tfrac{1}{2}y_j+\sum_{m=1}^{j}y_m\right] , \quad (4.28)$$

we can drop the quadratic terms in the y_k's if, as assumed, $\eta>1$ and obtain

$$P=1+\tfrac{1}{2}\sum_{n=1}^{\infty}(-1)^n\int_{-\infty}^{\infty}dx_1\int_{x_1}^{\infty}dx_2\cdots\int_{x_{n-1}}^{\infty}dx_n\int_0^{\infty}dy_1\cdots\int_0^{\infty}dy_n\left[\frac{2\Delta}{\hbar}\right]^{2n}\times\left[\cos\left[\frac{2vx_1y_1}{\hbar}\right]\cos[Q_1(y_1)]+\sin\left[\frac{2vx_1y_1}{\hbar}\right]\sin[Q_1(y_1)]\right]\exp[-Q_2(y_1)]\times\prod_{k=2}^{n}\cos\left[\frac{2vx_ky_k}{\hbar}\right]\cos[Q_1(y_k)]\exp[-Q_2(y_k)] . \quad (4.29)$$

We can then, upon observing that the integrand in part of the variables is a symmetric function, perform the integrals to obtain for the dominating contribution (as indicated by the time difference cutoff on the y integration)

$$P=1-\frac{1}{2}\left[\frac{2\Delta}{\hbar}\right]^2\int_{-\infty}^{\infty}dx\int_0^{\delta}dy\cos\left[\frac{2vxy}{\hbar}-\tilde{\omega}y\right]\exp\left[-\left[\frac{2\Delta}{\hbar}\right]^2\int_x^{\infty}dx_1\int_0^{\delta}dy_1\cos\left[\frac{2vx_1y_1}{\hbar}\right]\cos(\tilde{\omega}y_1)\right] , \quad (4.30)$$

where $\tilde{\omega}=\eta\omega_c^2$.

Rescaling the variables we have the expression

$$P=1-2\gamma\int_{-\infty}^{\infty}dx\int_0^{\delta\tilde{\omega}}dy\cos[(x-1)y]\exp\left[-4\gamma\int_x^{\infty}dx_1\int_0^{\delta\tilde{\omega}}dy_1\cos(x_1y_1)\cos(y_1)\right] \quad (4.31)$$

which can be expressed in terms of the sine integral

$$P=1-2\gamma\int_{-\infty}^{\infty}dx\left[\frac{d}{dx}\{\mathrm{si}[\delta\tilde{\omega}(x-1)]\}\right]\times\exp(2\gamma\{\mathrm{si}[\delta\tilde{\omega}(x-1)]+\mathrm{si}[\delta\tilde{\omega}(x+1)]\})\ . \quad (4.32)$$

Since $\delta\tilde{\omega}\gg 1$, the sine integral is approximately steplike

$$\sin(\delta\tilde{\omega}x)=-\int_{\delta\tilde{\omega}x}^{\infty}dt\frac{\sin t}{t}\cong-\pi[1-\Theta(x)] \quad (4.33)$$

and the derivative appearing in Eq. (4.32) is therefore a peaked function around $x=1$ with a width $1/\delta\tilde{\omega}$. We can therefore perform the final integration and obtain to order $1/\sqrt{\eta}$ the strong-coupling limit result

$$P=\exp(-2\pi\gamma)\ . \quad (4.34)$$

In the event of high temperature, the present estimation procedure using δ as the small time difference cutoff is no longer appropriate because of the temperature dependence of the function Q_2. The cutoff is then dependent on the temperature

$$\delta_T=\left[\eta\omega_c\frac{k_B T}{\hbar}\right]^{-1/2}$$

and, as we discuss in detail in the next section, we find the restriction on the temperature for the above estimation to be valid to be

$$k_B T<\hbar\omega_c\ . \quad (4.35)$$

The criterion for the strong-coupling limit result for the transition probability Eq. (4.34) to be valid is thus both the criteria (4.25) and (4.35). We note that the coupling to the bath does not appear explicitly in the expression Eq. (4.34) to lowest order in $1/\eta$, and that to leading order there is no influence of the coupling to the environment. Just as the weak influence of the environment in the slow-passage, low-temperature limit was the result of cancellation between the two opposing influences of the bath on the dynamics of the spin, the situation is the same in the present strong-coupling limit. In the time span δ, the cutoff set by the fluctuation part through the function Q_2, the systematic influence tends to weaken the influence of the environment as the terms containing Q_1 in time span δ execute many oscillations. The recovery of adiabaticity in the strong-coupling limit is thus again the result of cancellation between the opposing effects of the environment.

In dropping the quadratic terms in Eq. (4.28), it could appear that we must require $v<\eta^{3/2}\hbar\omega_c^2$. In view of the strong-coupling criterion, Eq. (4.25), this restriction on the sweeping speed v seems to suggest that the result Eq. (4.34) is not valid in the strong-coupling, fast-passage limit. However, in the fast-passage limit, the rapid oscillations of the functions containing v leads to absence of any influence of the environment in accordance with the fast-passage limit of Eq. (4.34). In Sec. VII we study the fast-passage limit quite generally reaching the conclusion that there is no influence of the environment in this limit. The result in the strong-coupling limit thus joins up smoothly with the result in the fast-passage limit. As a consistency check of our calculations, we note that, in the event the coupling strength η satisfies the inequalities

$$1<\eta<\gamma\omega_c\tau_{\mathrm{LZ}}\ , \quad (4.36)$$

we should, at least at zero temperature, verify that the results of the strong coupling and the adiabatic calculations coincide, as, in fact, they do. The temperature restriction Eq. (4.35) in the strong-coupling limit is just that $k_B T$ must not be large compared to the highest energy $\hbar\omega_c$ of the bath modes. In that event, we are in the high-temperature regime which we now turn to discuss. In the high-temperature limit we shall find that there is no cancellation between the different influences of the bath and therefore discuss this important point further.

V. THE HIGH-TEMPERATURE LIMIT

The investigation of the adiabatic limit in Sec. III showed that a raising of the temperature has a drastic effect on the transition probability even at temperatures small compared to the energy gap. This feature is also born out in the present section where we evaluate the asymptotic behavior of the transition probability in the high-temperature limit.

In the high-temperature limit we assume that the thermal fluctuations completely dominate over the quantum fluctuations so that we require that

$$k_B T>\hbar\omega_c\ . \quad (5.1)$$

In this limit we have, provided $\omega_c t<1$, the following expression for Q_2:

$$Q_2(t)=\frac{k_B T\eta}{\hbar}\omega_c t^2\ . \quad (5.2)$$

As already noted in the preceding section, under the assumption Eq. (5.1), the time difference cutoff is then no longer the one, δ, set by the quantum fluctuations, but the much smaller one, δ_T, set by the thermal fluctuations. An estimation procedure based on the cutoff δ_T and the form Eq. (5.2) for Q_2 requires, for consistency, $\omega_c\delta_T<1$ or, equivalently,

$$k_B T>\frac{\hbar\omega_c}{\eta}\ . \quad (5.3)$$

Although the expression Eq. (5.3) implies that we are in the opposite limit of strong coupling according to the preceding section, sufficiently weak coupling violates the high-temperature criterion Eq. (5.3). However, the weak-coupling limit can be dealt with perturbatively as we show in the next section.

Just as in the strong-coupling calculation of the preceding section, we start from the noninteracting blip approximation expression Eq. (4.18) for the transition probability, but now control the evaluation of the integrals by the time difference cutoff δ_T introduced by the exponential damping due to thermal fluctuations as appearing through the function Q_2.

The difference compared to the strong-coupling limit now appears, as the cutoff δ_T decreases with increase in temperature and, in fact, if we require

$$k_B T > \eta \hbar \omega_c \ , \tag{5.4}$$

is so short that the terms containing Q_1 complete no oscillations in the time span δ_T. Since Q_1 is zero at time zero $[Q_1(0)=0]$, we obtain, in the high-temperature limit, the following expression for the transition probability:

$$P = 1 + \tfrac{1}{2} \sum_{n=1}^{\infty} (-1)^n \left[\frac{2\Delta}{\hbar} \right]^{2n} \int_{-\infty}^{\infty} dx_1 \int_{x_1}^{\infty} dx_2 \cdots \int_{x_{n-1}}^{\infty} dx_n \int_0^{\infty} dy_1 \cdots \int_0^{\infty} dy_n \prod_{k=1}^{n} \cos\left[\frac{2v}{\hbar} y_k x_k \right] . \tag{5.5}$$

We note that, in the high-temperature limit, the term containing the function h in the expression Eq. (4.18) for the transition probability gives no contribution. The remaining integral in Eq. (5.5), upon noting that the integrand is symmetric in the x's, is elementary and we obtain, in the high-temperature limit, $k_B T > \hbar\omega_c$, $\hbar\omega_c/\eta$, $\eta\hbar\omega_c$, the transition probability

$$P = \tfrac{1}{2}[1 + \exp(-4\pi\gamma)] \ . \tag{5.6}$$

We note that the present result is consistent in a nontrivial manner with the result we shall obtain in the fast-passage limit (Sec. VII).

The result Eq. (5.6) implies that, at high temperatures, adiabaticity is lost even in the slow-passage limit. In fact, in the slow-passage limit, the transition saturates at an equal population of the two levels showing that adiabaticity is completely lost due to strong mixing between the levels.

The expression Eq. (5.6) for the transition probability has also been obtained in phenomenological studies of the dissipative Landau-Zener model. In Ref. 6, a short-time relaxation-type approximation was applied to the equation of motion of the reduced spin-density matrix and, in Ref. 16, a stochastic treatment was given.

As noted previously and discussed in the Appendix, the environment influences the dynamics of the primary degree of freedom, the spin, in two different ways. One is the causal influence, describe by the retarded bath propagator, which relates the average displacement of the bath coordinate to a disturbance. For a θ-function disturbance, we have the average displacement of the bath coordinate

$$\begin{aligned} \langle X(t) \rangle_\Theta &= \int_{-\infty}^{\infty} dt' D^R(t,t')\Theta(t') \\ &= \int_0^t dt' D^R(t,t') \ , \end{aligned} \tag{5.7}$$

the displacement to a unit disturbance acting in the time span t. The other influence is stochastic, as it is equivalent to treating the bath coordinate as a Gaussian fluctuating quantity with the bath correlation function D^K proportional to the correlator. The two influences, however, are not independent as they are related through the fluctuation-dissipation relation.

In the expansion series in the energy gap, the two influences appear, through the functions Q_1 and Q_2, as certain time averages, as seen from Eqs. (4.10) and (4.11). In terms of the displacement of the bath coordinate, we have, for the function Q_1,

$$Q_1(t) = \frac{1}{\hbar} \int_0^t dt' \langle X(t) \rangle_\Theta + t \int_0^{\infty} d\omega \frac{J(\omega)}{\omega} \ . \tag{5.8}$$

The second term in Eq. (5.8) is the polaroniclike renormalization of the energy. At times smaller than the fastest time characterizing the oscillators $t_c = 1/\omega_c$, the oscillators are not displaced as reflected in Q_1 by the first term in Eq. (5.8) being quadratic in time and the systematic influence is solely from the second, renormalization, term which is linear in time and introduces the time scale $t_r = 1/(\eta\omega_c)$ characterizing the bath.

The function Q_2,

$$Q_2(t) = \frac{4i}{\hbar^2} t \int_0^t dt' D^K(t') \ , \tag{5.9}$$

is determined by the correlation function of the fluctuations exerted by the bath and introduces the characteristic time over which the fluctuations are correlated; $t_c = 1/\omega_c$ at low temperatures and $t_T = \hbar/(k_B T)$ at high temperatures.

In terms of these characteristic times, the high-temperature limit corresponds to the relationship

$$t_T < t_r < t_c \ , \tag{5.10}$$

whereas the strong-coupling limit corresponds to the relationship

$$t_r < t_c < t_T \ . \tag{5.11}$$

At this point we should comment on the stochastic model of nonadiabatic processes of adsorbates of Ref. 8. In this work the dynamical processes in chemisorption is studied. The adsorbates are assumed to be interacting with the degrees of freedom of the substrate; that is, phonons or electron-hole pair excitations. The study of this physical system is performed by the use of exactly the model we are studying. In Ref. 8, a high-temperature form of the fluctuations is assumed and features like the cancellation property in the adiabatic limit cannot be noticed. Furthermore, one cannot trust the numerical results in parameter regimes that violate the assumed high-temperature condition; that is, $k_B T \lesssim \Delta$.

Within our microscopic treatment we are able to assess the region of validity of the phenomenological approaches and identify their phenomenological parameters. Comparing with our microscopic model, we see that the stochastic models of Refs. 6, 8, and 16 correspond to neglect of the systematic force of the bath; that is, neglecting terms involving the retarded bath propagator D^R; take the high-temperature form of the fluctuating force term, $k_B T > \hbar\omega_c$ and ω_c larger than remaining characteristic frequencies, and assume an ohmic spectral function

$$J(\omega)=\eta\omega e^{-\omega/\omega_c} \tag{5.12}$$

so that the fluctuating force term reduces to the white-noise form corresponding to

$$D^K(t)=-i\pi\eta k_B T\hbar\delta(t) \; . \tag{5.13}$$

We can therefore identify the phenomenological fluctuation amplitude parameters of Ref. 6 and the so-called dephasing time of Ref. 16 as determined by the combination $\hbar/\pi\eta k_B T$.

It should be recognized that the phenomenological approach is a crude and quite uncontrollable approximation for the dissipative dynamics of the spin. In contrast, we start from the noninteracting blip approximation expression and the intermediate equations in the two approaches look very different up until the final step at which they reduce to the same result, Eq. (5.6).

VI. PERTURBATIVE TREATMENT

In the calculation of the transition probability in the adiabatic limit, we did not explicitly exploit any weak-coupling restriction and, for instance, found a divergent result except for low temperatures $k_B T \le \Delta/4\gamma$ almost independently of the coupling strength. In this section we shall treat the effect of the environment on the system perturbatively and, by working explicitly in the coupling strength, we shall hereby achieve the possibility of exploring the weak-coupling but intermediate-temperature regime. As we shall show, at intermediate temperatures we are in a highly nonadiabatic regime.

To perform a weak-coupling calculation of the transition probability, we split the Hamiltonian

$$H(t)=H^0(t)+H_i \tag{6.1}$$

into a zeroth-order noninteracting part

$$H^0(t)=H_s(t)+H_B \tag{6.2}$$

and treat the interaction with the environment

$$H_i=\sigma_z X \tag{6.3}$$

as the perturbation.

The evolution operator corresponding to $H^0(t)$, that is, the two separate systems the spin and the bath, decomposes into a system and a bath part

$$\begin{aligned} U_0(t,t')&=T\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,H^0(\bar{t})\right] \\ &=U_s(t,t')U_B(t,t') \; , \end{aligned} \tag{6.4}$$

where the spin-system evolution is governed by

$$U_s(t,t')=T\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,H_s(\bar{t})\right] \tag{6.5}$$

and the bath by

$$U_B(t,t')=\exp\left[-\frac{i}{\hbar}H_B(t-t')\right] . \tag{6.6}$$

Expressing the transition probability in terms of quantities referring to the interaction picture with respect to the zeroth-order Hamiltonian $H^0(t)$, we then get

$$\begin{aligned} P=\mathrm{Tr}[\rho_i \tilde{V}^\dagger(\infty,-\infty)U_s^\dagger(\infty,-\infty) \\ \times P_\uparrow U_s(\infty,-\infty)\tilde{V}(\infty,-\infty)] \; , \end{aligned} \tag{6.7}$$

where the evolution operator in the interaction picture with respect to $H^0(t)$

$$\tilde{V}(t,t')=T\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}\,H_i^I(\bar{t})\right] \tag{6.8}$$

is specified by the Hamiltonian in the interaction picture

$$H_i^I(t)=U_0^\dagger(t,t_0)H_i U_0(t,t_0)=\sigma_z(t)X(t) \; , \tag{6.9}$$

where

$$\sigma_z(t)=U_s^\dagger(t,t_0)\sigma_z U_s(t,t_0) \tag{6.10}$$

and

$$X(t)=\exp\left[\frac{i}{\hbar}H_B(t-t_0)\right]X\exp\left[-\frac{i}{\hbar}H_B(t-t_0)\right] . \tag{6.11}$$

Introducing a complete set of spin states $|i\rangle$, $i=1,2$, we can express the probability P as

$$P=\mathrm{tr}\left[\rho_B \sum_{i,j}\langle\uparrow|V^\dagger(\infty,-\infty)|i\rangle U_{ij}\langle j|\tilde{V}(\infty,-\infty)|\uparrow\rangle\right] , \tag{6.12}$$

where the matrix elements of the spin evolution are given by

$$U_{ij}=\langle i|U_s^\dagger(\infty,-\infty)|\uparrow\rangle\langle\uparrow|U_s(\infty,-\infty)|j\rangle \; . \tag{6.13}$$

The matrix elements U_{ij} can be expressed in terms of the solutions of the Schrödinger equation for the system part

$$i\hbar\frac{d\psi}{dt}=H_s(t)\psi(t) \; . \tag{6.14}$$

Explicitly defining

$$\psi_1=\langle\uparrow|U_s(\infty,-\infty)|\uparrow\rangle \tag{6.15}$$

and

$$\psi_2=\langle\downarrow|U_s(\infty,-\infty)|\uparrow\rangle \; , \tag{6.16}$$

we can rewrite the transition probability P as

$$P=|\psi_1|^2\mathrm{tr}[\rho_B\langle\uparrow|\tilde{V}^\dagger(\infty,-\infty)|\uparrow\rangle\langle\uparrow|\tilde{V}(\infty,-\infty)|\uparrow\rangle]+(1-|\psi_1|^2)\mathrm{tr}[\rho_B\langle\uparrow|\tilde{V}^\dagger(\infty,-\infty)|\downarrow\rangle\langle\downarrow|\tilde{V}(\infty,-\infty)|\uparrow\rangle]$$
$$-2\,\mathrm{Re}\{\psi_1^*\psi_2^*\mathrm{tr}[\rho_B\langle\uparrow|\tilde{V}^\dagger(\infty,-\infty)|\uparrow\rangle\langle\downarrow|\tilde{V}(\infty,-\infty)|\uparrow\rangle]\}\;. \quad (6.17)$$

So far the treatment has been quite general, but we are now in a position from which we can calculate the transition probability P perturbatively in the coupling strength by expanding $\tilde{V}$, and to lowest order in the coupling we obtain

$$P=P_1+P_2+P_3\;, \quad (6.18)$$

$$P_1=|\psi_1|^2(1-2P_2)\;, \quad (6.19)$$

$$P_2=\frac{4i}{\hbar^2}\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2 D^{>}(t_1,t_2)\psi_1^*(t_1)\psi_2^*(t_1)\psi_1(t_2)\psi_2(t_2)\;, \quad (6.20)$$

$$P_3=-\frac{4}{\hbar^2}\mathrm{Im}\left[\psi_1^*\psi_2^*\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2[|\psi_1(t_1)|^2-|\psi_2(t_1)|^2]\psi_1(t_2)\psi_2(t_2)[2\theta(t_1-t_2)D^{>}(t_1,t_2)-D^{A}(t_1,t_2)]\right]\;, \quad (6.21)$$

where the advanced bath correlator is given by

$$D^A(t,t')=i\theta(t'-t)\langle[X(t),X(t')]\rangle \quad (6.22)$$

and satisfies the relation

$$D^A(t,t')=[D^R(t',t)]^*\;. \quad (6.23)$$

Here

$$\psi(t)=\begin{bmatrix}\psi_1(t)\\ \psi_2(t)\end{bmatrix}$$

denotes the solution of the matrix equation Eq. (6.14),[7,23] and accordingly the spin-up component $\psi_1(t)$ satisfies the equation

$$\left[\frac{d^2}{dt^2}+\left[i\frac{v}{\hbar}+(\Delta/\hbar)^2+(vt/\hbar)^2\right]\right]\psi_1(t)=0 \quad (6.24)$$

with the initial conditions

$$|\psi_1(-\infty)|=1,\quad i\hbar\left.\frac{d\psi_1}{dt}\right|_{t=-\infty}=v\lim_{t\to-\infty}[t\psi_1(t)] \quad (6.25)$$

and the spin-down component $\psi_2(t)$ satisfies the equation

$$\left[\frac{d^2}{dt^2}+\left[-i\frac{v}{\hbar}+(\Delta/\hbar)^2+(vt/\hbar)^2\right]\right]\psi_2(t)=0 \quad (6.26)$$

with the initial conditions

$$\psi_2(-\infty)=0,\quad i\hbar\left.\frac{d\psi_2}{dt}\right|_{t=-\infty}=v\lim_{t\to-\infty}[t\psi_2(t)]\;. \quad (6.27)$$

The solutions $\psi_1(t)$ and $\psi_2(t)$ of Eqs. (6.24)–(6.27) can be expressed in terms of parabolic cylinder functions $D_p(z)$ (Refs. 7 and 23)

$$\psi_1(t)=AD_{-i\gamma}\left[-\sqrt{2v/\hbar}\,t\exp\left[i\frac{\pi}{4}\right]\right]\;, \quad (6.28)$$

$$\psi_2(t)=-\sqrt{\gamma}\exp\left[i\frac{\pi}{4}\right]AD_{-i\gamma-1}\left[-\sqrt{2v/\hbar}\,t\exp\left[i\frac{\pi}{4}\right]\right]\;, \quad (6.29)$$

where the normalization constant A has the absolute value

$$|A|=\exp[-(\pi/4)\gamma]\;.$$

The expressions in Eqs. (6.15) and (6.16) equal $\psi_1(t)$ and $\psi_2(t)$, respectively, taken at time $t=\infty$.

A. The weak-coupling, slow-passage limit

Presently, we are not aware of relations that would give an exact evaluation of the integrals in Eqs. (6.20) and (6.21). However, in the slow-passage limit where the dimensionless parameter γ is large compared to one, and at temperatures $T>\Delta/\gamma k_B$, we can extract the leading order behavior. This can be achieved by using the asymptotic expansions of the parabolic cylinder functions.[24]

An integral in Eqs. (6.20) and (6.21) is divided into three parts guided by the possibility of asymptotic expansions of the parabolic cylinder functions. In terms of the dimensionless parameter for time $u=t\sqrt{2v/\hbar}$, the three parts are specified by the adiabatic parameter γ. In the region $u<-\sqrt{\gamma}$, the product of the two ψ's is a rapidly oscillating function, provided $\gamma>1$, since there we have

$$D_{-i\gamma}\left[-u\exp\left[i\frac{\pi}{4}\right]\right]=\exp\left[-i\frac{u^2}{4}-i\gamma\ln|u|+\frac{\pi}{4}\right]\times\{1+O[(1/\gamma)^2]\}\;, \quad (6.30)$$

$$D_{-i\gamma-1}\left[-u\exp\left[i\frac{\pi}{4}\right]\right]=|u|^{-1}\exp\left[\frac{\pi}{4}\gamma\right]\times\exp\left[-i\frac{u^2}{4}-i\frac{\pi}{4}-i\gamma\ln|u|\right]\times\{1+0[(1/\gamma)^2]\}\;. \quad (6.31)$$

The contributions to the integral from this region can therefore be neglected.

In the region $u\in(-\sqrt{\gamma},\sqrt{\gamma})$, we can use the expressions

$$D_{-i\gamma}\left[-u\exp\left[i\frac{\pi}{4}\right]\right]=\frac{1}{\sqrt{2}}\exp\left[i\sqrt{\gamma}u+\frac{\pi}{4}+\frac{i}{2}(1-\ln\gamma)\right]\times[1+0(1/\sqrt{\gamma})]\;, \quad (6.32)$$

$$D_{-i\gamma-1}\left[-u\exp\left[i\frac{\pi}{4}\right]\right] = \frac{1}{\sqrt{2\gamma}}\exp\left[i\sqrt{\gamma}u - i\frac{\pi}{4} + \frac{\pi}{4} + \frac{i}{2}(1-\ln\gamma)\right] \times[1+0(1/\sqrt{\gamma})] . \quad (6.33)$$

In this region the product of the two ψ's is therefore a simple harmonic and the integration can be performed.

In the region $u > \sqrt{\gamma}$, we have the asymptotic forms

$$D_{-i\gamma}\left[-u\exp\left[i\frac{\pi}{4}\right]\right] = \exp\left[-\frac{i}{4}u^2 - i\gamma\ln u - \frac{3\pi}{4}\gamma\right] \times[1+0(1/\gamma)] \quad (6.34)$$

and

$$D_{-i\gamma-1}\left[-u\exp\left[i\frac{\pi}{4}\right]\right] = \frac{\sqrt{2}\pi}{\Gamma(i\gamma+1)} \times\exp\left[\frac{i}{4}u^2 - i\gamma\ln u - \frac{\pi}{4}\right] \times[1+0(1/\gamma)] . \quad (6.35)$$

The product of the two ψ's can therefore be approximated by a constant and again the integration can be performed.

We therefore perform all the integrals approximately in the weak-coupling, slow-passage limit, $\gamma > 1$, and upon noting the cancellations among contributions to P_1, P_2, and P_3, we obtain the result

$$P = P_0 + \Delta P , \quad (6.36)$$

where P_0 is the exact transition probability in the absence of coupling

$$P_0 = |\psi_1|^2 = \exp(-2\pi\gamma) . \quad (6.37)$$

and the environment correction ΔP is given by

$$\Delta P = \frac{\pi}{2}\tau_{LZ} J(2\Delta/\hbar) n(2\Delta/\hbar) . \quad (6.38)$$

The expression Eq. (6.38) is valid for weak coupling and intermediate temperatures. We can thus easily obtain a prediction for the temperature region where the environment-dependent contribution ΔP is more important than the bare tunneling probability P_0 showing that the dominating contribution is from thermal transitions. We note that the result Eq. (6.38) is in accordance with a simple Golden Rule estimation, as the environment-induced transition probability is proportional to the time spent in the transition region, the effective coupling strength at the gap frequency, and the number of phonons at the gap energy.

The present calculation does not allow a discussion of the low-temperature regime $k_BT < \Delta/\gamma$ since we cannot control the correction terms beyond, in fact, temperatures $k_BT < \Delta/\ln\gamma$. However, we do not expect any qualitatively new temperature dependence in the intermediate regime so that the present result should join up smoothly with our low-temperature result of Sec. III, the stationary phase calculation. Similarly, we can not assess the high-temperature regime as the expression Eq. (6.38) increases linearly with temperature at high temperatures. However, as we showed in Sec. V, at high temperatures the transition saturates at an equal population of the two levels.

In view of the obtained results, we can now state the weak-coupling criterion quantitatively as

$$\eta < 1 . \quad (6.39)$$

In the weak-coupling limit the relevant high-temperature criterion is therefore the expression Eq. (5.3) as Eqs. (5.1) and (5.4) then are consequences thereof.

We note that weak coupling does not imply that the effect of the environment is small, as this strongly depends on the temperature. With these results we cover the whole temperature region in the slow passage, weak-coupling limit, and collect all the results below:

$$P = \begin{cases} P_0\exp[\mathcal{E}(T,\tau_{LZ})], & k_BT < \Delta/4\gamma , \\ P_0 + \pi\gamma\frac{\hbar}{\Delta}J(2\Delta/\hbar)\exp\left[-\frac{2\Delta}{k_BT}\right], & \Delta/4\gamma < k_BT < \Delta , \\ P_0 + \frac{\pi}{4v}J\left[\frac{2\Delta}{\hbar}\right]k_BT , & \Delta < k_BT < \min\left[\hbar\omega_c/\eta, \frac{2v}{\pi\eta\omega_c}\left[\frac{\hbar\omega_c}{2\Delta}\right]^s\right] , \\ \frac{1}{2}, & k_BT > \hbar\omega_c/\eta . \end{cases} \quad (6.40)$$

With the above results we have a complete picture of the slow-passage, weak-coupling limit. At low temperatures, $k_BT < \Delta/4\gamma$, the transition takes place through quantum tunneling without any modification due to the environment. The precursor effect at small temperatures $k_BT < \Delta/\gamma$ has, according to Eqs. (3.45) and (3.46), the form

$$P = \tilde{P}_0\left[1 + 2\pi^2\Gamma(s+3)\eta(\omega_c\tau_{LZ})^{1-s}\left[\gamma\frac{k_BT}{\Delta}\right]^{s+3}\right] . \quad (6.41)$$

At temperatures $\Delta/\gamma < k_BT < \Delta$, thermally assisted transitions across the energy gap dominates over quantum tunneling and at these intermediate temperatures we have the usual form of the transition probability for activation across an energy barrier. The crossover temperature separating quantum tunneling and thermal activation does not depend on the coupling strength (a feature analogous to the situation of tunneling out of a metastable state). At temperatures $k_BT > \Delta$, the transition probability increases linearly with temperature T and at higher temperatures

$$k_BT > \left[\hbar\omega_c/\eta, \frac{2v}{\pi\eta\omega_c}\left[\frac{\hbar\omega_c}{2\Delta}\right]^s\right] ,$$

we get saturation of the transition probability to the high-temperature value $\frac{1}{2}$.

VII. THE FAST-PASSAGE LIMIT

In this section we shall calculate the transition probability in the fast-passage limit where the Landau-Zener time is much smaller than the oscillation time of the two-level system. Using the expression for the transition probability, Eq. (6.18), valid to lowest order in the coupling, we can assess its properties in the weak-coupling and fast-passage limit where the dimensionless parameter γ is small compared to one. To do this we only have to observe that in the fast-passage limit we can use the following approximate (lowest order in Δ) solutions to Eqs. (6.24) and (6.26):

$$\psi_1(t)=\exp\left[-i\frac{v}{2\hbar}t^2\right] \tag{7.1}$$

and

$$\psi_2(t)=-i\frac{\Delta}{\hbar}\exp\left[i\frac{v}{2}t^2\right]\int_{-\infty}^{t}dt'\exp\left[-i\frac{v}{\hbar}t'^2\right] \tag{7.2}$$

and upon inserting these in the expression for P and performing partial integrations, we obtain, after collecting terms,

$$P=P_0-\frac{4}{\hbar^2}|\psi_1\psi_2|^2\langle B(\infty)B(\infty)\rangle+\frac{8}{\hbar^2}|\psi_1\psi_2|^2\langle B(t)B(t)\rangle -4\frac{\Delta^2}{\hbar^4}\int_{-\infty}^{\infty}dt_1\int_{-\infty}^{\infty}dt_2\langle B(t_1)B(t_2)\rangle \times\exp\left[i\frac{v}{\hbar}(t_1^2-t_2^2)\right], \tag{7.3}$$

where B is the integral of the bath operator

$$B(t)=\int_{-\infty}^{t}dt'X(t') . \tag{7.4}$$

The integral in Eq. (7.3) can be evaluated and, after noticing the complete cancellation between the lowest-order correction terms due to the environment, we obtain the result (valid for $\gamma<1$)

$$P=P_0=1-2\pi\gamma , \tag{7.5}$$

that is, there is no influence of the environment in the fast-passage limit.

This result can also be obtained, in fact, by a far less tedious calculation, by evaluating the transition probability in perturbation theory, doing lowest-order perturbation theory not as above in the coupling to the environment but only in the spin-flip term $\Delta\sigma_x$ of the original Hamiltonian Eq. (2.5) demonstrating that the result Eq. (7.5) is not restricted to weak coupling. In conjunction with the result for the strong-coupling limit, this shows that there is virtually no influence on the environment in the fast-passage limit. In order to perform the one-flip calculation we just note what it amounts in Eq. (3.34) for the transition probability, to perform the following substitutions:

$$vt/\varepsilon_t\rightarrow 1 \tag{7.6}$$

substitute the expression for the bare adiabatic phase

$$\int_{t'}^{t}d\bar{t}\;\varepsilon_{\bar{t}}\rightarrow v(t^2-t'^2) \tag{7.7}$$

and substitute for the amplitude factor

$$A\rightarrow-\left[\frac{\Delta}{\hbar}\right]^2 . \tag{7.8}$$

Then all integrations in Eq. (3.34) can be performed and we again obtain the result of Eq. (7.5). This result has also been obtained in Ref. 15. We obtain the result, however, without invoking the noninteracting blip approximation. The reason that we, in the fast-passage limit, do not have any effect of the bath at zero temperature is not as subtle as in the adiabatic limit where it depended on a cancellation between two opposing mechanisms. In the present limit both of these terms vanish (even at $T\neq 0$). The complete absence of influence of the environment in the fast-passage limit, that is, to the lowest order in the inverse sweeping rate, is only valid for the considered linear sweep model. In the fast-passage limit we therefore obtain the result, in agreement with the high-temperature strong-coupling results, respectively, that there is no influence of dissipation on the transition probability even at arbitrary temperatures and arbitrary coupling strength.

VIII. THE INFLUENCE OF DISSIPATION ON THE DECAY OF THE EXCITED STATE

In this section we shall briefly state the results for the decay of the excited state as the calculations parallel that of the previous sections. At a remote time we thus assume that our initial state is described by the initial statistical operator ρ_i',

$$\rho_i'=|\downarrow\rangle\langle\downarrow|\rho_B=P_\downarrow\rho_B \tag{8.1}$$

as the spin-down state at large negative times corresponds to the excited state. We then ask for the probability P' that the system in the far future has decayed to the ground state assuming the bath unobserved. This decay probability P' is then given by

$$P'=\mathrm{Tr}[\rho_i'U^\dagger(\infty,-\infty)P_\downarrow U(\infty,-\infty)] . \tag{8.2}$$

The calculation of the decay probability is equivalent to that of the excitation probability of the previous sections and we now state the results in various limits.

A. The slow-passage limit

Calculating the decay probability by the stationary phase method analogously to the calculation of Sec. III, we find that the two terms that cancelled for the case of the excitation transition, now instead add so that the decay probability P' is given by

$$P'=\tilde{P}_0\exp(\mathcal{E}') \tag{8.3}$$

with a nonvanishing exponent $\mathcal{E}'$ at zero temperature

$$\mathcal{E}'(T,\tau_{\rm LZ}) = \pi^2\tau_{\rm LZ}^2\int_0^\infty d\omega\, J(\omega)[n(\omega)+1]I_1^2(\omega\tau_{\rm LZ}) \ . \quad (8.4)$$

The transition probability at zero temperature is enhanced, in fact, except for spectra with a very small cutoff, $\omega_c = 1(2\tau_{\rm LZ})$, the expression is ultraviolet divergent. Due to strong spontaneous emission, adiabaticity is thus unattainable for the decay transition, where we start from the excited state. This result shows that, in the slow-passage limit, the decay probability has a discontinuity as function of the coupling strength at η equal to zero.

B. The fast-passage limit

In the fast-passage limit, $\gamma < 1$, we obtain for the decay transition, just as for the excitation transition, that there is no effect of the environment. To lowest order in γ, we have

$$P' = 1 - 2\pi\gamma \ . \quad (8.5)$$

This result is obtained both for a one-flip calculation and a more tedious calculation in the weak-coupling limit. In accordance with the result for the strong-coupling limit [see Eq. (8.10)], this shows that for the decay transition there is also no influence of the environment in the fast-passage limit, thus completely paralleling the situation for the excitation transition.

C. The weak-coupling limit

A perturbative calculation in the coupling strength of the decay probability P' gives, in the slow-passage limit, $\gamma < 1$, and at intermediate temperatures

$$\Delta/\gamma < k_B T < \hbar\omega_c/\eta \ ,$$

the result

$$P' = P_0' + \Delta P' \ , \quad (8.6)$$

where P_0' is the bare decay probability

$$P_0' = P_0 \quad (8.7)$$

and

$$\Delta P' = \pi\gamma\frac{\hbar}{\Delta}J\left[\frac{2\Delta}{\hbar}\right]\left[n\left[\frac{2\Delta}{\hbar}\right]+1\right] \ . \quad (8.8)$$

As to be expected, the only difference as compared with the excitation probability is that we, for the decay probability, have the additional effect of spontaneous emission. The strong enhancement of the decay probability due to the presence of the environment as indicated by Eq. (8.8) is consistent with the result of the investigation above of the slow-passage limit where strong spontaneous phonon emission leads to the absence of adiabaticity and here limits the range of validity of Eq. (8.8) to weak coupling or low temperatures.

D. The strong-coupling limit

The strong-coupling calculation for the decay probability is equivalent to that of Sec. IV and we obtain, to lowest order in $1/\sqrt{\eta}$ at temperatures $k_B T < \hbar\omega_c$, the result

$$P' = 1 - \exp(-2\pi\gamma) + \exp(-4\pi\gamma) \ . \quad (8.9)$$

In analogy with the result for the excitation transition Eq. (4.34), the coupling strength does not appear explicitly in the expression Eq. (8.9) to lowest order in $1/\eta$. However, in contrast to the case of the excitation transition, the result does not reduce to that of the bare transition probability. For the decay transition the previously found strong influence of the environment due to phonon emission should result in a decay probability close to one. This is indeed reflected in the result Eq. (8.9), as for all values of γ, the expression is close to one, except for a sharp dip at the value $\gamma = (\ln 2)/2\pi$. We note that the result Eq. (8.9) agrees in a nontrivial manner with the result in the fast-passage limit that there is no influence of the environment.

E. The high-temperature limit

The expression for the decay probability differs only from the expression for the excitation probability Eq. (4.18) in the respect that the term containing the function h appears with the opposite sign. However, as this term is negligible in the high-temperature limit, $k_B T > \hbar\omega_c$, $\hbar\omega_c/\eta$, $\eta\hbar\omega_c$, we have

$$P' = \tfrac{1}{2}[1 + \exp(-4\pi\gamma)] \quad (8.10)$$

as a result of the strong mixing between the levels dominating this limit and correspondingly the same expression as for the excitation probability.

IX. APPLICATIONS

We shall now use the obtained results to estimate the influence of a dissipative environment on the transition processes in a few of the various physical systems we mentioned in the Introduction. The present choice of examples should be regarded as illustrating the experimental relevance of the obtained results, rather than giving an exhaustive account for all the relevant physical phenomena mentioned in the Introduction.

A. Macroscopic quantum tunneling

In the context of macroscopic quantum tunneling,[25] we now show that the dynamics of the model we have studied can represent the behavior of a rf SQUID in a time-dependent external flux. The electromagnetic behavior of a SQUID is described in terms of the magnetic flux Φ threading the superconducting ring[26]

$$H(P_\Phi,\Phi) = \frac{P_\Phi^2}{2C} + V(\Phi) \ , \quad (9.1)$$

where $P_\Phi = C\dot{\Phi}$ is the conjugate variable to the flux and the potential energy V is given by

$$V(\Phi) = \frac{(\Phi-\Phi_{\rm ex})^2}{2L} - \frac{I_c\Phi_0}{2\pi}\cos\left[2\pi\frac{\Phi}{\Phi_0}\right] \ . \quad (9.2)$$

The SQUID parameters are capacitance C, self inductance L, and critical current I_c, Φ_{ex} is the external flux, and $\Phi_0=h/(2e)$ the superconducting flux quantum. For values of the external flux Φ_{ex} close to half a flux quantum, the potential V has the shape depicted in Fig. 3. For the case where the system parameters and the temperature are such that the following conditions are met:

$$\tilde{\varepsilon},\hbar\omega_{1,2} > \varepsilon,\Delta,k_B T \ , \tag{9.3}$$

we are effectively dealing with a two-state system. The level spacings ω_1, ω_2, and energy off sets ε and $\tilde{\varepsilon}$ are depicted in Fig. 3 and Δ is the tunneling matrix element. Incidentally, we note that the conditions (9.3) are identical to the conditions for the observability of macroscopic quantum coherence,[25,27–29] however, for the situation we consider, we do not need to have exactly half a flux quantum as bias.

The truncated two-level Hamiltonian describing the SQUID under the conditions (9.3) is

$$H=\varepsilon\sigma_z+\Delta\sigma_x \ , \tag{9.4}$$

where

$$\varepsilon=\frac{\Phi_c}{L}\Phi_{ex} \tag{9.5}$$

and Φ_c is the smallest nonzero solution of the equation

$$\frac{\Phi_c}{L}=I_c\sin\left[2\pi\frac{\Phi_c}{\Phi_0}\right] . \tag{9.6}$$

For the situation where the external flux are changed at a constant rate through the value of half a flux quantum, the SQUID is described by our system Hamiltonian of Eq. (2.1). The tunneling matrix element Δ is given by[29]

$$\Delta=2\sqrt{3}\hbar\omega_0\left[\frac{S_0}{2\pi\hbar}\right]^{1/2}\exp\left[-\frac{S_0}{\hbar}\right] , \tag{9.7}$$

where the exponent

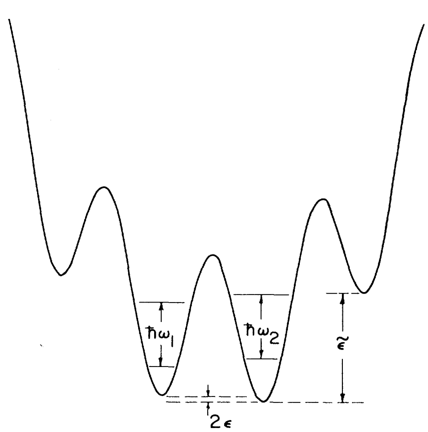

FIG. 3. The potential $V(\Phi)$ of a SQUID ring as a function of the flux.

$$S_0=\frac{16}{3}\frac{\Delta U}{\omega_0} \tag{9.8}$$

is given in terms of the barrier height ΔU and the small oscillation frequency ω_0 of the wells as determined by the potential V. For a variety of experimentally achievable SQUID parameters, we have predicted the tunneling rate of the flux for differing experimentally realizable cases depending on the rate of change of the external flux as well as temperature region.

B. Zener tunneling in solids

We can use our model to estimate qualitatively the effect of dissipation on the Zener transition for typical parameters in a two-band model of a semiconductor. Here we typically have a energy gap of order 1 eV, so that Δ is of order 1 eV. With a unit cell of size 5 Å and an electric field of order 10^6 V/cm, we then have a value of the slowness parameter γ of the order of 100, so that we are certainly in the slow-passage limit (basically because we have such a large energy gap),[30] and the zero-temperature tunneling probability is therefore extremely small. The characteristic temperature $\Delta/\gamma k_B$ is of order 100 K, so at temperatures below 25 K, we are in the adiabatic regime. To estimate the typical effect at these temperatures, we put $k_BT=\Delta/4\gamma$ and, although we can have many orders of magnitude of increase in the transition probability, the absolute value is still minute. If we consider a superlattice, the value of γ is typically at least an order of magnitude smaller than for the semiconductor case, due to the much smaller band gap, and therefore in a regime where there can be substantial influence of electron-phonon and possibly electron-electron interaction on the Zener tunneling.

C. Level crossing and the solar neutrino puzzle

As an example of the wide range of applications of the model we consider, we shall briefly discuss the relevance of our results to the solar neutrino puzzle which is the puzzle that only a fraction of the expected electron neutrinos produced inside the sun is observed at Earth.[4,31] As an electron neutrino produced inside the sun moves through the sun, it interacts through the electroweak interaction with electrons and a conversion from electron neutrino to muon neutrino can take place. An electron neutrino created at high electron density in the center of the sun will then, in the adiabatic limit, evolve into a muon neutrino which cannot be detected thus explaining the deficit in the number of the observed electron neutrinos. Assuming a two-flavor model, electron and muon neutrinos,[4,31] and a slowly varying density of electrons in the sun, we obtain Eq. (6.14) for neutrino propagation through the sun (assuming level crossing to take place, in accordance with the solar radius being of the order of the neutrino vacuum wavelength), where the spin is now interpreted as the neutrino flavors and our sweeping rate

$$v=\sqrt{2}G_F\left|\frac{dN}{dt}\bigg|_{t=0}\right| \tag{9.9}$$

is proportional to the change in electron density at the resonance

$$\left.\frac{dN}{dt}\right|_{t=0}$$

(taken to be at time $t=0$), and the electroweak interaction constant G_F, and Δ is the difference between the free-space mass squares of the neutrinos. For typical values we obtain that the slow-passage limit is appropriate, and the probability for a nonadiabatic transition of the electron neutrino to stay electron neutrino is given by the Landau-Zener expression Eq. (6.37).

The question we wish to consider is whether thermal fluctuations in the electron density in the sun will change the bare estimate. The fluctuations in the (free) electron gas corresponds to an ohmic spectral density $J(\omega)=\eta\omega$, where $\eta=(G_F m N^{1/3}/\hbar^2)^2$. So even though the temperature in the sun is 10^6 K, the effect of thermal fluctuations calculated according to formula Eq. (6.38) will thus be insignificant. The smallness of the weak interaction constant thus results in negligible effects from electronic density fluctuations. However, if a magnetic moment[31] is attributed to the neutrinos, the much stronger electromagnetic interaction could come into play as the fluctuating magnetic field from the fluctuating electronic current density would couple to such a magnetic moment.

X. SUMMARY AND CONCLUSION

We have performed an analytical study of the dissipative Landau-Zener model. Analytical results have been obtained by performing expansions in all the possible dimensionless variables of the model and a comprehensive understanding of the dissipative dynamics has emerged.

Let us first discuss the excitation transition and the question of adiabaticity. In contrast to the situation in the absence of an environment where adiabaticity only depends on the dimensionless parameter γ being large, characterizing the speed with which the levels cross, the coupling to an environment restricts adiabaticity to the low-temperature or strong-coupling regime. For weak or moderate coupling, the temperature restriction is strongest as the adiabatic criterion in this regime is

$$k_B T \leq \hbar/2\tau_{\mathrm{LZ}}, \quad \gamma > 1, \quad \eta \leq 1 \ . \tag{10.1}$$

In the strong-coupling limit adiabaticity is recovered once the following criteria are met:

$$\sqrt{\eta} > 1, \quad \gamma > \tfrac{1}{2}\pi, \quad k_B T < \hbar\omega_c \ . \tag{10.2}$$

We have shown that adiabaticity in both limits owes its existence to compensation between the dissipative and fluctuation influence of the bath. In particular, at zero temperature we found that there is no influence of the environment due to exact compensation between the two influences and showed that this is a property unique to the standard linear-sweep model.

Continuing the discussion of the slow-passage limit from the low-temperature end, the strong influence of an increase in temperature renders the transition nonadiabatic so that above the adiabatic low-temperature regime where the transition is dominated by quantum tunneling, without any modification due to the presence of the environment, a nonadiabatic intermediate regime appears dominated by thermally assisted transitions. Finally, at high temperatures the transition saturates at equal population of the levels, signifying that adiabaticity is completely lost. The transition probability thus exhibits a monotonic increase as function of temperature.

Quite contrary we find the following behavior of the transition probability as a function of coupling strength η: In the absence of coupling, of course, only quantum tunneling can take place; with increasing coupling strength, the transition probability increases, at first linearly with a coefficient that depends on the temperature regime under consideration. Since we in the strong-coupling limit have recovered adiabaticity, in fact with complete suppression of effects of the environment, we conclude that the transition probability is a nonmonotonic function of the coupling strength η, whose initial value for zero coupling and limiting value for large-coupling strength equals the bare transition probability and takes on a maximum value at intermediate-coupling strength.

In the fast-passage limit we have found that there is virtually no influence on the excitation transition of the environment; that is, to lowest order in the dimensionless parameter γ, we do not find any environment-dependent correction to the transition probability. At intermediate values of γ the whole range of possibilities can be achieved ranging from no influence of the environment on the transition to almost equal population depending on the actual temperature and coupling strength.

Let us now discuss the decay transition. We found that, for physically relevant environments, the adiabatic limit does not exist for this transition in the linear-sweep model, not even at zero temperature. Except for the fast-passage limit and the high-temperature limit, the transition is dominated by strong spontaneous emission. In view of Eqs. (8.8) and (8.10), we observe that, for very weak coupling, the decay transition probability exhibits nonmonotonic behavior as function of temperature and Eqs. (8.6) and (8.9) indicate a monotonic increase as function of the coupling strength. In the fast-passage limit we found that, just as in the case of the excitation transition, there is no influence of the environment. In the high-temperature limit we found the same expression for the decay probability as for the excitation probability in accordance with the complete loss of memory of the initial state in this limit.

We have established, on the basis of a first-principles calculation, that previous phenomenological approaches to the quantum dynamics of level crossing in a dissipative environment is a high-temperature limit where compensation between the influences of the environment is absent. In conclusion, we have demonstrated that, in dissipative quantum dynamics, one encounters a variety of behaviors even for a simple model as the one presently studied. In the absence of the environment, the model is exactly solvable, whereas in the presence of the environment the problem becomes nontrivial. Nevertheless, we have showed that the analytical treatment is sufficiently exhaustive that a complete description of the dissipative quantum dynamics can be given. For the sake of completeness we have compiled our results in the following table.

TABLE I. SUMMARY OF RESULTS. Hamiltonian $H=vt\sigma_z+\Delta\sigma_x+\sigma_z\sum_\alpha\lambda_\alpha(a_\alpha^\dagger+a_\alpha)+\sum_\alpha\hbar\omega_\alpha(a_\alpha^\dagger a_\alpha+\frac{1}{2})$, $\gamma\equiv\Delta^2/2\hbar v$, $\tau_{\rm LZ}\equiv\Delta/v$. Spectral function $J(\omega)\equiv(4/\hbar^2)\sum_\alpha\lambda_\alpha^2\delta(\omega-\omega_\alpha)$. When estimation is needed, we take $J(\omega)=\eta\omega(\omega/\omega_c)^{s-1}\exp(-\omega/\omega_c)$. P is the excitation transition probability, transition from ground state to excited state. P' is the decay transition probability, transition from excited state to ground state.

Transition probabilities	Validity regimes
$P=\exp(-2\pi\gamma)$	$\eta=0$
$P'=\exp(-2\pi\gamma)$	γ arbitrary
$P=\left[\frac{\pi}{4}\right]^2\exp(-2\pi\gamma)\exp\left[\pi^2\tau_{\rm LZ}^2\int_0^\infty d\omega\, J(\omega)n(\omega)I_1^2(\omega\tau_{\rm LZ})\right]$	$k_BT\le\frac{\Delta}{4\gamma}$, $\eta\le 1$
$P'=\left[\frac{\pi}{4}\right]^2\exp(-2\pi\gamma)\exp\left[\pi^2\tau_{\rm LZ}^2\int_0^\infty d\omega\, J(\omega)[n(\omega)+1]I_1^2(\omega\tau_{\rm LZ})\right]$	$\tau_{\rm LZ}>\frac{2\hbar}{\Delta}$
$P=\exp(-2\pi\gamma)$	$k_BT<\hbar\omega_c$, $\sqrt{\eta}>1$
$P'=1-\exp(-2\pi\gamma)+\exp(-4\pi\gamma)$	γ arbitrary
$P=\pi\gamma\frac{\hbar}{\Delta}J\left[\frac{2\Delta}{\hbar}\right]n\left[\frac{2\Delta}{\hbar}\right]$	$\frac{\Delta}{4\gamma}<k_BT<\min\left[\hbar\omega_c/\eta,\frac{2v}{\pi\eta\omega_c}\left[\frac{\hbar\omega_c}{2\Delta}\right]^s\right]$
$P'=\pi\gamma\frac{\hbar}{\Delta}J\left[\frac{2\Delta}{\hbar}\right]\left[n\left[\frac{2\Delta}{\hbar}\right]+1\right]$	$\eta<1$ $\tau_{\rm LZ}>\frac{2\hbar}{\Delta}$
$P=\frac{1}{2}[1+\exp(-4\pi\gamma)]$	$k_BT>\hbar\omega_c/\eta$, $\eta\hbar\omega_c$, $\hbar\omega_c$
$P'=\frac{1}{2}[1+\exp(-4\pi\gamma)]$	γ arbitrary
$P=1-2\pi\gamma$	k_BT and η arbitrary
$P'=1-2\pi\gamma$	$\tau_{\rm LZ}<\frac{2\hbar}{\Delta}$

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APPENDIX: DERIVATION OF THE FORMAL PERTURBATION EXPRESSION IN Δ^2 FOR THE TRANSITION PROBABILITY P

In this appendix we show how to arrive at the formal perturbation expansion in Δ^2 for the excitation probability P using the real-time nonequilibrium generating functional technique. In Sec. II we used the method, in particular, in connection with the adiabatic calculation. Besides supplying the technical details of the method, we shall discuss the characteristic features of dissipative quantum dynamics.

We split the Hamiltonian in Eq. (2.5) into off-diagonal and diagonal parts in spin space

$$H(t)=H_d(t)+H_\Delta\ ,\quad H_d(t)=vt\sigma_z+H_B+H_i\ ,\quad H_\Delta=\Delta\sigma_x\ . \tag{A1}$$

The expression for the transition probability is given in Eq. (2.11) and since $H_d(t)$ is diagonal in spin space, we have

$$P=\mathrm{tr}[\rho_B\langle\uparrow|V_\Delta^\dagger(\infty,-\infty)|\uparrow\rangle\langle\uparrow|V_\Delta(\infty,-\infty)|\uparrow\rangle]\ , \tag{A2}$$

where V_Δ is the evolution operator in the interaction picture with respect to $H_d(t)$

$$V_\Delta(t,t')=T\exp\left[-\frac{i}{\hbar}\int_{t'}^t d\bar{t}\,H_\Delta(\bar{t})\right] \tag{A3}$$

so that

$$H_\Delta(t)=U_d^\dagger(t,-\infty)H_\Delta U_d(t,-\infty)\ , \tag{A4}$$

where

$$U_d(t,t')=T\exp\left[-\frac{i}{\hbar}\int_{t'}^t d\bar{t}\,H_d(\bar{t})\right]\ . \tag{A5}$$

With the given initial and final condition on the spin value (spin up), both matrix elements in Eq. (A2) will, upon expanding the exponential, contain an even number of transitions, so, for example,

$$\langle\uparrow|V_\Delta(\infty,-\infty)|\uparrow\rangle=\sum_{n=0}^\infty\left[-i\frac{\Delta}{\hbar}\right]^{2n}\int_{-\infty}^\infty dt_1\int_{-\infty}^{t_1}dt_2\cdots\int_{-\infty}^{t_{2n-1}}dt_{2n}\,W(t_1,\ldots,t_{2n})\ , \tag{A6}$$

where

$$W(t_1,\ldots,t_{2n})=U_1^\dagger(t_1,-\infty)U_{-1}(t_1,t_2)U_{+1}(t_2,t_3)\cdots U_{-1}(t_{2n-1},t_{2n})U_1(t_{2n},-\infty) \tag{A7}$$

and

$$U_{\pm 1}(t,t')=T\exp\left[-\frac{i}{\hbar}\int_{t'}^{t}d\bar{t}(\pm v\bar{t}+H_B\pm H_i)\right]. \tag{A8}$$

are operators on the bath states, being different by reflecting the virtual state of the spin.

Combining with a similar expression for the complex conjugate matrix element, we have traced out the spin degree of freedom and can express the transition probability as

$$P=\sum_{m,n=0}^{\infty}(-1)^{n+m}\left[\frac{\Delta}{\hbar}\right]^{2(n+m)}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{t_{2n-1}}dt_{2n}\int_{-\infty}^{\infty}d\tilde{t}_1\cdots\int_{-\infty}^{\tilde{t}_{2m-1}}d\tilde{t}_{2m}\,G(t_1,\ldots,t_{2n};\tilde{t}_1,\ldots,\tilde{t}_{2m}), \tag{A9}$$

where the closed-time-path integral G,

$$G(t_1,\ldots,t_{2n};\tilde{t}_1,\ldots,\tilde{t}_{2m})=\left\langle T_c\exp\left[-i/\hbar\int_c d\tau\,\zeta_m^n(\tau)[v\tau+X(\tau)]\right]\right\rangle, \tag{A10}$$

has the form of a generating functional in $\zeta_m^n(\tau)$, which is short for the function of contour time τ as well as the times where the perturbation acts (spin flips) $(t_j)_{j=1,\ldots,2n}$, $(\tilde{t}_j)_{j=1,\ldots,2m}$,

$$\zeta_m^n(\tau)=\zeta_m^n(\tau;t_1,\ldots,t_{2n};\tilde{t}_1,\ldots,\tilde{t}_{2m}),$$

and has the form

$$\zeta_m^n(\tau)=\begin{cases}\zeta_1^n(\tau)=1-2\sum_{k=1}^{2n}(-1)^k\theta(\tau-t_k), & \tau \text{ on upper branch},\\ \zeta_2^m(\tau)=1-2\sum_{k=1}^{2m}(-1)^k\theta(\tau-\tilde{t}_k), & \tau \text{ on lower branch}.\end{cases} \tag{A11}$$

The structure of the sign changes for $\zeta_m^n(\tau)$ is depicted in Fig. 4 and corresponds to the diagonal and off-diagonal elements of the reduced spin-density matrix. The bath operator $X(t)$ in Eq. (A10) is in the interaction picture as given in Eq. (3.19).

As in Sec. II we can invoke Wick's theorem to obtain the generating functional for the bath in terms of the "history of the spin motion" ζ_m^n and according to Eqs. (3.22) (3.26), and (3.27), and a reintroduction of real time, we obtain

$$\begin{aligned}Z[\zeta_m^n]&=\left\langle T_c\exp\left[-i/\hbar\int_c d\tau\,\zeta_m^n(\tau)X(\tau)\right]\right\rangle\\ &=\exp\left[-\frac{i}{2\hbar^2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'[\zeta_1^n(t)D_{11}(t,t')\zeta_1^n(t')+\zeta_2^m(t)D_{22}(t,t')\zeta_2^m(t')\right.\\ &\qquad\left.-\zeta_1^n(t)D_{12}(t,t')\zeta_2^m(t')-\zeta_2^m(t)D_{21}(t,t')\zeta_1^n(t')]\right],\end{aligned} \tag{A12}$$

where we have introduced the Green's functions

$$D_{12}(t,t')=-i\langle X(t')X(t)\rangle=D^{<}(t,t'), \tag{A13}$$

$$D_{21}(t,t')=-i\langle X(t)X(t')\rangle=D^{>}(t,t'), \tag{A14}$$

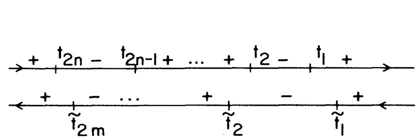

FIG. 4. The sequence of sign changes for $\zeta_m^n(\tau)$.

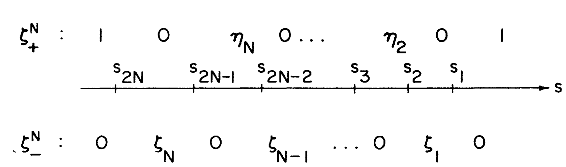

FIG. 5. The typical sequence of values attained by ζ_+^N and ζ_-^N.

$$D_{22}(t,t')=-i\langle \tilde{T}[X(t)X(t')]\rangle=-[D_{11}(t,t')]^* \ . \tag{A15}$$

Here $\tilde{T}$ denotes antitime ordering and D_{11} is defined in Eq. (3.33). Z is the scalar product of two amplitudes for two possible spin histories in the presence of the interaction with the environment (expansion of the reduced density matrix for the spin degree of freedom).

We can split the exponent into real and imaginary parts and obtain

$$Z[\zeta^{(n,m)}]=\exp\left[-\frac{i}{\hbar^2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'[2\zeta_-^{(n,m)}(t)D^R(t,t')\zeta_+^{(n,m)}(t')+\zeta_-^{(n,m)}(t)D^K(t,t')\zeta_-^{(n,m)}(t')]\right] , \tag{A16}$$

where we have defined

$$\zeta_\pm^{(n,m)}(t)=\tfrac{1}{2}[\zeta_1^n(t)\pm\zeta_2^m(t)] \ . \tag{A17}$$

In this representation the history of the spin motion is recounted by $\zeta_\pm^{(n,m)}$ whose alternating series of 0 and ± 1 are depicted in Fig. 5.

In the present approach products of amplitudes are described jointly by the introduction of the closed time path as evident in Eq. (A10). Accounting for the effects of the environment couples the upper and lower branch. We note the following Hermitian property resulting from interchanging the interaction times on the upper and lower branches:

$$\zeta_\pm^{(n,m)}(t)=\pm\zeta_\pm^{(m,n)}(t) \ . \tag{A18}$$

Pairing up these terms, each other's complex conjugate, displays explicitly that the transition probability P is real. The functions $\zeta_\pm^{(n,m)}$ take on the values ± 1 and 0, and change value at all interaction times t_k and $\tilde{t}_k$'s. To deal with the intertwined time orderings of the two sets, we denote by $(s_k)_{k=1,\dots,2(n+m)}$, a given time ordering on the real axis of the combined sets and note that all possible time orderings correspond to the following possible choices:

$$[\zeta_-^{(n,m)}(s),\zeta_+^{(n,m)}(s)]=\begin{cases}(0,1), & s<s_{2N}\\ (\pm 1,0), & s_{2N}<s<s_{2N-1}\\ (0,\pm 1), & s_{2N-1}<s<s_{2N-2}\\ \vdots & \vdots\\ (\pm 1,0), & s_2<s<s_1\\ (0,1), & s_1<s\end{cases} \ . \tag{A19}$$

Since $\zeta_\pm^{(n,m)}$ refers to the combined set, we can introduce the shorthand notation $\zeta_\pm^N$, where N is the number $N=n+m$. When $\zeta_+^N(s)=\pm 1$, then $\zeta_-^N(s)=0$ and vice versa; the final and initial values for a numerically large value of s are fixed by the choice of initial and final spin states. We can therefore express $\zeta_\pm^N$, as depicted in Fig. 5, in terms of the sets of numbers $(\eta_k)_{k=2,\dots,N}$; $(\zeta_k)_{k=1,\dots,N}$, where η_k and ζ_k only take values ± 1 [the explicit dependence on $s_1,\dots,s_{2N}$ and (η_k) and (ζ_k) is suppressed],

$$\zeta_+^N(s)=\sum_{k=2}^{N}\eta_k[\theta(s-s_{2k-1})-\theta(s-s_{2k-2})]+\theta(s-s_1)+\theta(s_{2N}-s) \ , \tag{A20}$$

$$\zeta_-^N(s)=\sum_{k=1}^{N}\zeta_k[\theta(s-s_{2k})-\theta(s-s_{2k-1})] \ . \tag{A21}$$

The expression for the transition probability can then be written as

$$P=\sum_{N=0}^{\infty}(-1)^N\left[\frac{\Delta}{\hbar}\right]^{2N}\int\limits_{s_1>\cdots>s_{2N}} ds_1\cdots\int ds_{2N}\sum_{[\eta_k,\zeta_k]}\exp\left[\frac{-i}{\hbar^2}\int_{-\infty}^{\infty}dt\int_{-\infty}^{\infty}dt'\zeta_-^N(t)D^K(t,t')\zeta_-^N(t')\right]$$
$$\times\cos\left[2\int_{-\infty}^{\infty}dt\,\zeta_-^N(t)\left[vt/\hbar+\frac{1}{\hbar^2}\int_{-\infty}^{\infty}dt'D^R(t,t')\zeta_+^N(t')\right]\right] . \tag{A22}$$

Expression (A22) for the transition probability has the following interpretation: The interaction with the bath provides a systematic force on the spin described by the retarded bath propagator D^R, which adds to the external force, and a fluctuating force with correlations described by the Keldysh bath propagator D^K (corresponding to treating X not as an operator but as a fluctuating quantity).

The spin history is recounted by $\zeta_\pm^N$ describing when the reduced spin-density matrix is diagonal and off diagonal. When the density matrix is diagonal, $\zeta_+^N\neq 0$, the bath records this and reacts back with a systematic, history-dependent influence ζ_B^N which is equal to the average displacement of the bath variable in the presence of the "force" ζ_+^N,

$$\zeta_B^N(t)=\langle X(t)\rangle_{\zeta_+^N}=\frac{1}{\hbar}\int_{-\infty}^{\infty}dt'D^R(t,t')\zeta_+^N(t') \ . \tag{A23}$$

When the density matrix is off diagonal, $\zeta_-^N\neq 0$, the bath records it and the suppression of the quantum interference terms by the fluctuating force term is reflected by the property of the prefactor, the exponential being less than 1. The relationship between the two types of influences required by the fluctuation-dissipation theorem is expressed by the equilibrium property of the bath propagators

$$D^{K}(\omega)=2i\,\mathrm{Im}D^{R}(\omega)\coth(\hbar\omega/2k_{B}T)\ . \qquad (A24)$$

Here $D^{R,K}(\omega)$ are the Fourier-transformed functions

$$D^{R,K}(\omega)=\int d(t-t')e^{i\omega(t-t')}D^{R,K}(t,t') \qquad (A25)$$

and the imaginary part of the retarded function $D^{R}(\omega)$ is given in terms of the spectral function J by the relation

$$\mathrm{Im}D^{R}(\omega)=-\frac{\pi\hbar^2}{4}\mathrm{sgn}\omega J(|\omega|)\ . \qquad (A26)$$

Performing the integration in Eq. (A22) for given spin histories (a given sequence of switching times), and performing the (η_k) summation, we obtain the expression of Leggett *et al.*,[21] which is given in Eq. (4.1).

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