Competition between relaxation and external driving in the dissipative Landau-Zener problem

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Abstract

We study Landau-Zener transitions in a dissipative environment by means of the quasiadiabatic propagator path-integral scheme. It allows to obtain numerically exact results for the full range of the involved parameters. We discover a nonmonotonic dependence of the Landau-Zener transition probability on the sweep velocity which is explained in terms of a simple physical picture. This feature results from a nontrivial competition between relaxation processes and the external sweep and is not captured by perturbative approaches. In addition to the Landau-Zener transition probability, we study the excitation survival probability and also provide a qualitative understanding of the involved competition of time scales.

Keywords: Landau-Zener problem, driven dissipative quantum mechanics, quasiadiabatic propagator path integral

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1. Introduction

The transition dynamics in a quantum two-level system with a time-dependent Hamiltonian varying such that the energy separation of the two diabatic states is a linear function of time is a central problem since the early days of quantum mechanics. It is commonly denoted as the Landau-Zener (LZ) problem, although it has been solved independently by Landau [1], Zener [2], Stückelberg [3] and Majorana [4] in 1932 (for a more detailed discussion of the differences between the four approaches, we refer the interested reader to a paper by Di Giacomo and Nikitin [5]). Nonadiabatic transitions at avoided level crossings are at the heart of many dynamical processes throughout physics and chemistry. They have been extensively studied both theoretically and experimentally in, e.g., spin flips in nanomagnets [6], solid state artificial atoms [7, 8, 9], nanocircuit QED [10, 11], adiabatic quantum computation [12], the dynamics of chemical reactions [13], and in Bose-Einstein condensates in optical lattices [14]. Also the nonequilibrium dynamics of glasses at low temperatures is dominated by the transition dynamics of avoided level crossings [12, 13, 17, 18].

In the pure Landau-Zener problem, two quantum states interact by a constant tunneling matrix element ∆0. A control parameter is swept through the avoided level crossing at a constant velocity v, such that the energy gap between the two diabatic states depends linearly on time. The Landau-Zener problem addresses the case when the system starts in the lower energy eigenstate in the infinite past and asks for the probability of finding the system in the lower energy eigenstate in the infinite future (a Landau-Zener transition). Certainly, for infinitely slow variation of the energy difference v → 0, the adiabatic theorem states that no transition between energy eigenstates will occur, since at any moment of time, the system will always be in an instantaneous eigenstate of the Hamiltonian. For v ≠ 0, the probability $P_0$ for no transition is described by the Landau-Zener formula $P_0(v, \Delta_0) = 1 - \exp[-\pi \Delta_0^2/(2v)]$.

Most experimental investigations, on the one hand, actually deal with more complex systems than two-state systems and, on the other hand, do...
not necessarily start in the ground state. In close
proximity around the avoided crossing in most cases
only the two crossing states are important to de-
scribe the dynamics. However, in general in such
an approximate system we also have to deal with
the system being initially in the excited state. In
the pure Landau-Zener problem the probability to
end up in the ground (excited) state when starting
in the ground (excited) state are identical due to
symmetry.

However, in any physical realization, a quantum
system is influenced by its environment leading to
relaxation and phase decoherence during time evolu-
tion [20, 21]. At low temperatures when the en-
vironmental fluctuations are not thermally occu-
pied, the Landau-Zener probability \( P \) (to end up
in the ground state when starting in the ground
state) should hardly be influenced since no phonons
are available for the system to be in the excited
state at asymptotically long times. However, sponta-
aneous emission is possible even at lowest tempera-
tures and the excitation survival probability \( Q \) (to
end up in the excited state when starting in the ex-
cited state) is expected to decrease when the sys-
tem has the time to relax during the driving. Thus
especially at low driving speeds, the excitation sur-
vival probability will be reduced since the system
will decay, while the purely Landau-Zener mechanism
predicts full survival of excitations when driving
through an avoided crossing at low speeds.

The dissipative Landau-Zener problem received
a lot of attention [22, 23, 24, 25, 26, 27, 28, 29] in
the past 25 years due to its relevance for controlled
quantum state preparation which became experi-
mentally feasible in many physical realizations. Al-
though the full problem is analytically unsolved,
many limiting cases are analytically tractable and
numerical approaches are available. Usually a dis-
sipative environment causes fluctuations of the en-
ergies of the diabatic states (longitudinal or dia-
ogonal system-bath coupling) but occasionally the
environments can also cause transitions between the
diabatic states (transversal system bath coupling).
In this work, we focus on the more common case of
longitudinal coupling. The transversal coupling has
been treated in Refs. [21, 22] for zero temperature.

In the limit of very fast sweeps (nonadiabatic
driving), a thermal heat bath has been shown not
to influence the Landau-Zener probability. This fol-
lows consistently from all approaches (for the cor-
responding limiting conditions of the other free pa-
rameters) [22, 23, 24, 25, 26, 27, 28, 29, 30].

At low temperatures, the Landau-Zener (or,
equivalently, ground state survival) probability \( P \)
to end up in the ground state when starting in the
ground state is only influenced little by a diagno-
sally coupled bath. This was first shown by Ao and
Rammer [24]. Kayanuma [22, 23] showed before
that in the limit of slow fluctuations of the diabatic
energies (as might be caused by a diagonally cou-
pled bath at low temperatures), the Landau-Zener
probability is not modified. At zero temperature, a
diagonally coupled bath has strictly no influence on
the Landau-Zener probability, as has been shown by
Wubs et al. [23]. This is true not only for bosonic
but also for spin environments [26]. In contrast,
transversely coupled baths lower the Landau-Zener
probability even at zero temperatures [25] and their
effects depend on the details of the bath character-
istics [26].

The strong damping limit can be reached in
two ways. For large coupling between system and
bath and finite temperatures, Ao and Rammer [24]
have shown that again a diagonally coupled bath
does not influence the Landau-Zener probability.
Conversely, in the high temperature limit under
adiabatic conditions (i.e., slow sweeps), the two
states are driven to equal population, \( P = P_{SD} = \frac{1}{2}(1 - \exp(-\pi \Delta J / \nu)) \). This has first been shown by
Kayanuma [22, 23] for large and fast fluctuations
and later by Ao and Rammer [24]. Pokrovsky and
Sun [28] have extended Kayanuma’s result to trans-
versely coupled environments.

For the experimentally important parameter
range of slow (adiabatic) sweeps and interme-
iate temperatures but only weakly coupled envi-
enments, Pokrovsky and Sun [28], Kayanuma and
Nakayama [27], and Ao and Rammer [24] each give
approximate solutions of the influence of the envi-
ronmental fluctuations on the Landau-Zener prob-
ability. Using the numerically exact quasidiabatic
propagator path-integral (QUAPI) technique, we
recently described the Landau-Zener probability in
the full parameter space [29]. For small sweep ve-
cocities and medium to high temperatures, we have dis-
covered non-monotonic dependencies on the sweep
velocity, temperature, coupling strength and cut-off
frequency which were not included in the previous
approximate solutions. This behavior can be un-
derstood in simple physical terms as a nontrivial
competition between relaxation and Landau-Zener
driving.

The direct influence of environmental fluctua-
tions on the dynamics of a driven two-state sys-
tem is much more pronounced when the system is initially prepared in the excited state since spontaneous emission is even possible at zero temperature. Accordingly, the excitation survival probability \( Q \) (to end up in the excited state having started in the excited state), which is without environment strictly identical to the Landau-Zener probability, is strongly modified for all temperatures and bath coupling strengths \[24, 27\]. Although experimentally highly relevant, the excitation survival probability received much less attention. In the limit of fast (nonadiabatic) sweeps, no influence of a bath is expected \[24, 27\]. In the high temperature limit under adiabatic conditions (slow sweeps), the two states are again driven to equal population, \( Q_{SD} = P_{SD} = \frac{1}{2}(1 - \exp(\pi \Delta_0^2/v)) \) \[24, 27\].

Thus, in both limits the excitation survival probability is identical to the Landau-Zener probability, \( Q = P \). However, this is quite different at intermediate and low temperatures since spontaneous emission drastically changes the excitation survival probability. Ao and Rammer \[24\] were the first to remark that in the limit of weak system-bath coupling, a discontinuity occurs. In the limit of strong coupling and low temperature, Kayanuma and Nakayama \[27\] find another simple analytical expression, \( Q_{ac} = P_0(1 - P_0) \) with \( P_0 \) being the Landau-Zener probability without environment. Both, Kayanuma and Nakayama \[27\] and Ao and Rammer \[24\] give approximate solutions to the experimentally important parameter range of slow (adiabatic) sweeps and intermediate temperatures, but only weakly coupled environments. Nevertheless, this parameter range is still largely unexplored.

Beyond these direct approaches, the dissipative Landau-Zener problem was discussed in many more facets. Not being able to give a full review of all works, we just mention in passing that Moyer \[3\] discussed the Landau-Zener problem for decaying states involving complex energy eigenvalues \[30\]. Extensions to three-state systems \[31\] or circuit QED problems \[32\] have been made recently. Finally, we also mention that spin environments in the context of Landau-Zener transitions have been discussed by Garanin et al. \[33\].

In this paper, we investigate the dissipative Landau-Zener problem in the full parameter range of sweep velocities, temperatures, damping strengths and cut-off frequency by means of the quasidiabatic propagator path-integral (QUAPI) \[34, 35, 36, 37, 38\]. It allows to include nonadiabatic as well as non-Markovian effects yielding numerically exact results. In the next section we introduce the basic model. In the third section we discuss the time-dependent occupation probability of the two states during a Landau-Zener transition and in the following section we focus on the asymptotic populations discussing the Landau-Zener (ground state survival) and the excitation survival probabilities in dependence of the sweep velocities, temperatures, damping strengths and cut-off frequency. We show that interesting features arise due to a competition between time scales associated to the Landau-Zener sweep and to dissipative transitions. Finally, we conclude with a short summary.

2. Model

A quantum mechanical two-state system which shows an avoided energy level crossing when driven is described by the Landau-Zener Hamiltonian \( (\hbar = 1) \)

\[
H_{LZ}(t) = \frac{\Delta_0}{2} \sigma_z + \frac{vt}{2} \sigma_z,
\]

with the tunneling matrix element \( \Delta_0 \) and the energy gap between the diabatic states \( v t \), changing linearly in time with sweep velocity \( v \). Here, \( \sigma_{x,z} \) are Pauli matrices and the diabatic states are the eigenstates (\( \downarrow \) and \( \uparrow \)) of \( \sigma_z \). Asymptotically at times \( |t| \gg \Delta_0/v \), the diabatic states coincide with the momentary eigenstates of \( H_{LZ} \). Figure 1 plots the eigenenergies of \( H_{LZ} \) (full lines) which show an avoided level crossing with minimal splitting \( \Delta_0 \) and the energies of the diabatic states (dashed lines) which form an exact crossing as a function of time.

The Landau-Zener problem asks for the probability \( P_0 \) of the system to end up in the ground state at \( t = +\infty \), having started in the ground state at \( t = -\infty \) (the corresponding one to end in the excited state is given as \( 1 - P_0 \)). Its exact solution dates back to the year 1932 \[31, 32, 33, 34\] and is given by

\[
P_0(v, \Delta_0) = |\langle \uparrow (\infty) | \downarrow (-\infty) \rangle|^2 = 1 - \exp \left( -\frac{\pi \Delta_0^2}{2v} \right).
\]

The excitation survival probability \( Q_0 \) to end up in the excited state at \( t = +\infty \), having started in the excited state at \( t = -\infty \) is strictly identical, \( Q_0 = P_0 \) for the coherent two-state problem.

To include environmental fluctuations on Landau-Zener transitions, we couple \( H_{LZ} \) diago-
nally to a harmonic bath \([20,21]\), yielding

\[
H(t) = H_{\text{LZ}}(t) - \frac{\alpha}{2} \sum_k \lambda_k (b_k^\dagger b_k + b_k b_k^\dagger) + \sum_k \omega_k \left( b_k^\dagger b_k + \text{c.c.} \right)
\]

(3)

with the bosonic annihilation/creation operators \(b_k, b_k^\dagger\). The bath influence is captured by the spectral function \(J(\omega) = 2\omega \exp(-\omega/\omega_c)\), for which we choose here for definiteness an Ohmic form with the cut-off frequency \(\omega_c\) and the coupling strength \(\alpha\) \([20,21]\). The Landau-Zener probability for the dissipative problem \(P = \text{Tr}\{ | \uparrow \rangle \langle \uparrow | U_\infty | \downarrow \rangle \langle \downarrow | U_\infty^{-1} \}\) with the time evolution operator \(U_\infty = T \exp[-i \int_0^\infty dt H(t)]\) as well as the excitation survival probability \(Q = \text{Tr}\{ | \downarrow \rangle \langle \downarrow | U_\infty | \uparrow \rangle \langle \uparrow | U_\infty^{-1} \}\) are now functions not only of \(\Delta_0\) and \(v\), but also of \(\alpha, \omega_c\) and the temperature \(T\). In the following, we use \(\omega_c = 10\Delta_0\) unless specified otherwise.

3. Time dependent occupation probabilities

In this section, we explicitly consider the time-dependence of the population of the diabatic state \(| \uparrow \rangle\) at any instant of time \(t\), having started in \(| \downarrow \rangle\) with probability one. This is given by

\[
P(t) = \text{Tr}\{ | \uparrow \rangle \langle \uparrow | U_t | \downarrow \rangle \langle \downarrow | U_t^{-1} \}\equiv P(t)\]

(4)

with the time evolution operator \(U_t = T \exp[-i \int_0^t dt' H(t')]\). Note that at asymptotic times, this quantity coincides with the standard Landau-Zener probability \(P = P(t \to \infty)\). Note furthermore that \(P(t)\) is the tunneling probability at any instant of time. Here, the dynamics of the quantum two-level system is described in terms of the time evolution of the reduced density matrix \(\rho(t) = \text{Tr}_B\{U_t \rho_0 U_t^{-1}\}\), starting from a total initial density matrix \(\rho_0 = \rho_S \otimes e^{-H_B/T}/Z_B\), where \(\rho_S\) is the density operator of the quantum two-level system and \(H_B\) denotes the bath Hamiltonian which is assumed to be decoupled at \(t_0 = -\infty\) (which is in practice set to zero) and instantly switched on directly afterwards. Moreover, \(Z_B = \text{Tr}\{ e^{-H_B/T} \}\) with \(k_B = 1\). \(\rho(t)\) is obtained after tracing over the bath degrees of freedom. We calculate \(\rho(t)\) using the numerically exact quasiadiabatic propagator path-integral \([34,35,36,37,38]\) scheme. For details of the iterative technique, we refer to previous works \([34,35,36,37,38]\).

In brief, the algorithm is based on a symmetric Trotter splitting of the short-time propagator \(K(t_{k+1}, t_k)\) for the full Hamiltonian into a part depending on the system Hamiltonian and a part involving the bath and the coupling parts. The short time propagator describes time evolution over a Trotter time slice \(\Delta t\). This splitting is of course exact in the limit \(\Delta t \to 0\) but introduces a finite Trotter error to the splitting, which has to be eliminated by choosing \(\Delta t\) small enough such that convergence is achieved. On the other hand, the bath degrees of freedom generates correlations being non-local in time. For any finite temperature, these correlations decay exponentially fast at asymptotic times, thereby defining the associated memory time scale. QUAPI now defines an object called the reduced density tensor, which lives on this memory time window and establishes an iteration scheme in order to extract the time evolution of this object. Within the memory time window, all correlations are included exactly over the finite memory time \(\tau_{\text{mem}} = K\Delta t\) and can safely be neglected for times beyond \(\tau_{\text{mem}}\). Then, the memory parameter \(K\) has to be increased, until convergence is found. Typical values, for which convergence can be achieved for our problem, are \(K \leq 12\) and a reasonable choice is \(\Delta t \sim (0.1 - 0.2)/\Delta_0\). The two strategies to achieve convergence, namely decreasing \(\Delta t\) and at the same time increasing the considered memory time \(\tau_{\text{mem}} = K\Delta t\), are clearly increasing both the needed \(K\) which results in severe demands considering that the needed computer power grows exponentially with \(K\). Nevertheless convergent results can be obtained in a wide range of parameters.

Fig. 1 shows the population \(P(t)\) vs. time for different temperatures for a fixed sweep velocity \(v = 0.02\Delta_0^2\) in the weak coupling regime \(\alpha = 0.0016\). We start in the infinite past with \(P(t = -\infty) = 0\) as the state \(| \downarrow \rangle\) is fully populated, see Fig. 1. The Landau-Zener sweep reaches the minimal gap at \(t = 2500/\Delta_0\). Approaching this point, \(P(t)\) starts to increase. For larger temperatures, this increase is less pronounced than for lower temperatures. This is shown more explicitly in Fig. 1 where the corresponding derivative \(dP(t)/dt\) is shown. Note that this quantity may be viewed as tunneling rate for the dissipative Landau-Zener transition. It is naturally more pronounced at low temperatures. Increasing the speed of the Landau-Zener sweep, the population \(P(t)\) of the \(| \downarrow \rangle\) state shows some transient oscillatory dynamics before a stationary value is reached (results not shown). We would like to point out that the iterative QUAPI approach...
by construction allows the access to the full time-dependent Landau-Zener transition. In the following, we focus on the stationary populations at asymptotic times without discussing how the stationary state is reached in all studied parameter configurations.

4. Landau-Zener and excitation survival probability

In this section, we turn to the asymptotic populations and study the Landau-Zener and the excitation survival probabilities.

4.1. Landau-Zener probability at weak coupling

Figure 4 shows the Landau-Zener probability $P$ versus sweep velocity $v$ for different temperatures and for weak coupling, $\alpha = 0.0016$. Clearly the regime with large velocities, $v \gg \Delta_0^2$ is distinguishable from a regime with small velocities (adiabatic regime) $v \lesssim \Delta_0^2$. At low temperatures one expects no sizable influence of the bath [27, 22, 23] which should vanish totally at $T = 0$ [25, 27]. This is confirmed by our numerical results. For small $v$ and low temperatures, $T \lesssim \Delta_0$, we find $P \sim 1$, and thus unmodified compared to the pure quantum mechanical Landau-Zener result $P_0$ (solid line). For increasing velocity, the Landau-Zener probability decreases rapidly and there is hardly any temperature effect in the considered temperature range, see Fig. 4. This observation agrees with results by Kayanuma and Nakayama who determined the Landau-Zener probability in the limit of high temperatures, $P_{SD} = \frac{1}{2}(1 - \exp(-\pi \Delta_0^2/v))$ [27, 22, 23] (dot-dashed line), assuming dominance of phase decoherence over dissipation. For large velocities, $P_{SD}$ decreases as the pure Landau-Zener probability, $P_{SD} \sim P_{LZ} \sim \frac{1}{2} \pi \Delta_0^2/v$, and accordingly no sizable temperature effect is expected.

In the experimentally most relevant parameter range of intermediate to high temperatures, $T > \Delta_0$ and small sweep velocities, $v < \Delta_0^2$, we find (as reported before [24]) a nontrivial and unexpected behavior of $P$. Besides an overall decrease of $P$ with increasing temperature, we find (at fixed $T$) for decreasing velocity first a maximum of $P$ at $v_{\text{max}} \lesssim \Delta_0^2$, then a minimum at $v_{\text{min}}$ and finally again an increase. For decreasing temperatures, $v_{\text{min}}$ decreases, and $P(v_{\text{min}})$ increases. For high temperatures $T \geq 500\Delta_0$, our data follow nicely the predictions by Kayanuma and Nakayama [27, 22, 23].

This nonmonotonic behavior cannot be described in terms of perturbative approaches. Ao and Rammer derived temperature-dependent corrections to the Landau-Zener probability for low temperatures [24]. They report an onset temperature $T_o \propto 1/v$, above which temperature affects $P$. Thus, at larger velocities, the decrease of $P$ due to increasing temperature starts at higher temperatures. This is in line with our findings of the maximum in $P(v)$, but it does not account for the minimum and the subsequent increase of $P$ for smaller $v$. In the limit of high temperatures, $P_{SD} \rightarrow 1/2$ for $v < \Delta_0^2$. Thus, $P_{SD}$ captures the decrease of $P$ in Fig. 4 with increasing temperature, but it does not account for the nonmonotonic behavior for decreasing $v$.

In Fig. 5 we compare our data (triangles for $P$ (top) and circles for $Q$ (bottom)) for $T = 4\Delta_0$ and $\alpha = 0.0016$ with the result of Ao and Rammer (dotted lines). In fact, the latter describes qualitatively the maximum both for $P$ and $Q$, but fails quantitatively. Similarly, we were not able to match either Eq. (54) of Ref. [27] (dashed line in Fig. 5) nor Eq. (40) of Ref. [28] (dash-dash-dotted line in Fig. 5) with our exact data, see Fig. 5. Both describe a reduction of the Landau-Zener probability with increasing temperature but neither the maximum nor the subsequent minimum in the behavior versus $v$ is predicted correctly.

4.2. Physical picture

The observed behavior can be understood within a simple physical picture realizing that the bath induces relaxation as main effect, whose time scale can compete with the Landau-Zener sweep velocity. Since initially the system is in the ground-state, only absorption can occur, if an excitation with energy $\Delta_t = \sqrt{\Delta_0^2 + (vt)^2}$ exists in the bath spectrum and is thermally populated. Since $\Delta_t$ (slowly) changing with time, relaxation can only occur during a time window $|t| \leq \frac{1}{2} t_r$ with the resonance time

$$t_r = \frac{2}{v} \sqrt{\Delta_0^2 - \Delta_c^2},$$

(5)

in which the energy splitting fulfills the condition $\Delta_t \leq \Delta_c = \min\{T, \omega_c\}$ [39] as illustrated in Fig. 1. In order for relaxation processes to contribute, the (so far unknown) relaxation time $\tau_r$ must be shorter than $t_r$.

For large sweep velocities, $t_r \ll \tau_r$, relaxation is negligible and no influence of the bath is found as expected. In the opposite limit, $t_r \gg \tau_r$, relaxation will dominate and the two levels will at any time
adjust their occupation to the momentary $\Delta_t$ and $T$. Once $\Delta_T \geq \Delta_s$, relaxation stops since no spectral weight of the bath modes is available and the corresponding “critical” Landau-Zener probability can be estimated as

$$P_c = \frac{1}{\pi} \left[ 1 + \tanh \left( \frac{\Delta_c}{2 T} \right) \right].$$

For small but finite $v$, equilibration is retarded. The two levels need the finite relaxation time to adjust their occupation to the momentary $\Delta_t$ and $T$. In this time, however, $\Delta_t$ might exceed $\Delta_c$, and then relaxation is not possible anymore. Thus equilibrium is reached for an energy splitting in the past $\Delta_T < \Delta_s$, with $t' < t_c$ and $t_c$ the time when $\Delta_t = \Delta_c$. Accordingly, $P$ increases with decreasing $v$ since $\Delta_t$ changes slower and $P(v \to 0) \leq P_c$, as observed in Fig. 4. In Fig. 6 (main), we plot the Landau-Zener probability $P(v = 0.005 \Delta_0^2)$ (blue diamonds) for the smallest investigated sweep velocity and compare it with $P_c$ of Eq. 6 (blue full line).

Relaxation will maximally suppress the Landau-Zener transition when both time scales coincide, leading to a minimum of $P$ at $v_{\text{min}}$ given by the condition

$$t_r(v_{\text{min}}) = \tau_r(T, \alpha, \omega_c).$$

(7)

Within the resonance time window, $|t| \leq \frac{1}{4} t_r$, only a single phonon absorption is likely. We thus can assume equilibration associated to a time-averaged energy splitting $\langle \Delta_R \rangle = \frac{1}{t_r} \int_0^{t_r} dt \Delta_t \approx \max\{\Delta_t/2, \Delta_0\}$ and a resulting Landau-Zener probability

$$P_{\text{min}} = \frac{1}{\pi} \left[ 1 + \tanh \left( \frac{\Delta_R}{2 T} \right) \right] = P(v_{\text{min}}).$$

(8)

Subsequently, there is a maximum for a sweep velocity between $v_{\text{min}} < v_{\text{max}} < \Delta_0^2$. Fig. 4 (main) shows the QUAPI data $P(v_{\text{min}})$ (black circles) vs. $T$ together with $P_{\text{min}}$ given in Eq. 8 (black dashed line).

For a fixed time and for weak coupling, we can estimate the decay rate out of the ground state using Golden Rule, $\tau^{-1}(t) = \pi \alpha (\Delta_t^2/\Delta_s) \exp(-\Delta_t/\omega_c)n(\Delta_t)$ with the Bose factor $n(\Delta_t) = \left[ \exp(\Delta_t/T) - 1 \right]^{-1}$. For the time-dependent Landau-Zener problem at slow sweep velocities, we may assume that the bath sees a time-averaged two-level system and thus estimate the relaxation rate $\tau_r^{-1}$ by using the time-averaged energy splitting $\overline{\Delta_R}$, i.e.,

$$\tau_r^{-1} \approx \pi \alpha \frac{\Delta_0^2}{\Delta_r} \exp(-\overline{\Delta_R}/\omega_c)n(\overline{\Delta_R}).$$

(9)

For increasing temperature, relaxation becomes faster, and, accordingly, the condition for $v_{\text{min}}$, Eq. 7, leading to

$$v_{\text{min}} = 2^{5/2} \Delta_0^2 \Delta_0^2$$

(10)

is fulfilled for larger velocities. Qualitatively this picture describes the temperature dependence of $v_{\text{min}}$ observed in the inset of Fig. 6. We plot $v_{\text{min}}$ (red squares) taken from the data of Fig. 6 and $v_{\text{min}}$ according to Eq. 10. In detail, given the section-wise definition of the parameters $\Delta_t$ and $\overline{\Delta_R}$, the agreement in Fig. 6 is rather satisfactory, keeping in mind that there are no adjustable parameter involved.

4.3. Excitation survival probability at weak coupling

Figure 7 shows the excitation survival probability $Q_s$ versus sweep velocity $v$ for different temperatures and for weak coupling, $\alpha = 0.0016$. As for the Landau-Zener probability, the regime with large velocities, $v \gg \Delta_0^2$ is distinguishable from a regime with small velocities (adiabatic regime) $v \ll \Delta_0^2$. For large sweep velocities, the excitation survival probability decreases rapidly. There is no sizable difference to the undamped case for all the considered temperatures, as expected in the high temperature limit, $Q_{SD} (v \gg \Delta_0^2)$ as well as in the low temperature limit for weak coupling $Q_0 (v \gg \Delta_0^2)$ and strong coupling $Q_{\infty} (v \gg \Delta_0^2)$ since

$$Q_{\infty} (v \gg \Delta_0^2) \approx Q_0 (v \gg \Delta_0^2) \approx Q_{SD} (v \gg \Delta_0^2) \approx P_0 (v \gg \Delta_0^2) \approx \frac{1}{8} \frac{\Delta_0^2}{v}.$$

(11)

At low temperatures, $T \lesssim \Delta_0$, no sizable influence of the bath is found as the data in Fig. 7 for $T = 0.01 \Delta_0$ almost coincide with the data for $T = 0.5 \Delta_0$ (and even more so for data at $T = 0.05 \Delta_0$ and $T = 0.1 \Delta_0$ not shown in the figure). However, for all temperatures we find the excitation survival probability to peak for sweep velocities between $0.1 - 1 \Delta_0^2$ and a strong decrease for lower sweep velocities as predicted by 24 and 27. For small sweep velocities relaxation of the excited state takes place and thus reduces the excitation survival probability as soon as the relaxation time becomes comparable or shorter than the resonance
time. Due to spontaneous emission relaxation is present at all temperatures. Furthermore we would expect in this picture that only at temperatures $T \geq \Delta_0$ the relaxation time becomes shorter due to induced emission by excited phonons and thus only for $T \geq \Delta_0$ a temperature effect should be visible in the excitation survival probability. This is confirmed by the results in Fig. 7. Consistent with our simple physical picture introduced in the last section is that the sweep velocity of the sharp reduction of the excitation survival probability coincides roughly with the minimum in Fig. 4 for $T > \Delta_0$. It, as well, shifts to larger $v$ for increasing temperatures.

Taking the sweep velocity $v_a = v[Q(T) = \frac{1}{2}\Delta_0]$ (with temperature fixed) as a measure for the sweep velocity of the sharp reduction, we expect $v_a$ to be the sweep velocity for which the resonance time (Eq. (6)) coincides with the relaxation time, up to a prefactor $f_a$ of order one which is due to the arbitrary definition of $v_a$, i.e.,

$$f_a \tau_r(v_a) = \tau_{d,r}.$$  

(12)

The inverse decay time of the excited state is now given as

$$\tau_{d,r}^{-1} \approx \frac{\Delta_r^2}{\Delta_c} \exp(-\frac{\Delta_c}{\omega_c}) \left[ 1 + n(\Delta_c) \right].$$  

(13)

Since thermal occupation is no limiting factor for the decay of the excited state, we have that $\Delta_c = \omega_c$ and thus $\Delta_r = \omega_c/2$. Fig. 8 plots $v_a$ (black squares) versus temperature which nicely shows a temperature behavior $\sim \left[ 1 + n(\Delta_c) \right]$. The black line marks the result of the best fit of Eq. (12) with the fitting parameter $f_a \approx 3.04$, confirming again the good agreement between our numerical data and our simple physical picture.

In the high temperature limit, $Q \to P_{SD}$ 24 27. In our data, we observe that the peak in $Q$ decreases with increasing temperature and $Q$ at smallest investigated sweep velocity increases with increasing temperature. Both features are in agreement with the expectation in the high temperature limit. For the smallest investigated sweep velocity, the relaxation time should exceed the resonance time by far and thus we expect within our simple picture that the system fully relaxes towards the momentarily equilibrium until the energy splitting exceeds $\Delta_c = \omega_c$. This yields the condition

$$Q_c = \frac{1}{2} \left[ 1 - \tanh \left( \frac{\Delta_c}{2T} \right) \right].$$  

(14)

The inset of Fig. 8 compares $Q_c$ with $Q(v = 0.005\Delta_0^2)$ extracted from Fig. 7 and again shows satisfactory agreement.

The excitation survival probability is numerically much harder to determine than the Landau-Zener probability. For example, at the sweep velocities $v = 0.005\Delta_0^2$ our data did not converge for temperatures below $T = 4\Delta_0$ and hence is not shown. According to our physical picture, the main effects of the bath occur during the resonance time window. Outside of it, only multi-phonon processes can occur, which are strongly suppressed due to the weak coupling. This directly affects our numerical scheme which is thus not sensitive to the very long times needed to perform a Landau-Zener experiment (from $t = -\infty$ to $t = +\infty$). In contrast, for the Landau-Zener probability all relaxation effects outside the resonance time window are additionally suppressed by thermal occupation numbers of the phonons. This effect does not influence the excitation survival probability due to spontaneous decay. These multi-phonon processes outside the resonance time window are, however, processes which need long memory in the bath and may thus be critical for convergence of our numerics. We should emphasize that our simple physical picture even explains our stronger numerical efforts to obtain converged results for the excitation survival probability.

In summary, at weak coupling our simple physical picture explains qualitatively fully and quantitatively satisfactorily both the Landau-Zener as well as the excitation survival probability. Both are unmodified by the dissipative effects of the environment for large velocities, $v \gg \Delta_0^2$. For slow velocities $v \lesssim \Delta_0^2$, both are strongly influenced due to relaxation where a striking difference emerges since the excited state can relax by spontaneous emission whereas the ground state can only absorb a phonon when one is thermally occupied. Thus the Landau-Zener probability at vanishing temperature is unmodified by the presence of the bath whereas the excitation survival probability is strongly altered, i.e. decreases rapidly for sweep velocities smaller than $v_a$ determined by the competition of driving and relaxation.

4.4. Medium to strong couplings

Surprisingly, our simple picture still holds qualitatively for stronger damping, when the Golden Rule is not expected to hold. Increasing $\alpha$ enhances relaxation and $\tau_r$ and $\tau_{d,r}$ decrease. Thus, the
sweep velocity of the minimum in the Landau-Zener probability as well as \( v_a \) in the excitation survival probability increase for larger coupling strengths \( \alpha \) (at fixed temperature). This is confirmed by Fig. 9 where \( P \) is shown for the same temperatures as in Fig. 4 but for a larger value of \( \alpha = 0.02 \). Fig. 10 shows the corresponding excitation survival probability for \( \alpha = 0.02 \). The minimum of \( P \) and \( v_a \) for \( Q \) are still observable for \( \alpha = 0.02 \) for temperatures \( \Delta_0 \leq T \leq 4\Delta_0 \). At higher temperatures, only a shoulder remains for \( P \) in Fig. 9 and \( Q \) in Fig. 11 does not exceed 1/2 anymore. Results for \( P \) and \( Q \) for even stronger coupling \( \alpha = 0.2 \) are shown in Fig. 11. For \( \alpha = 0.2 \), the local extrema in \( P \) disappear, but a monotonic growth of \( P \) with decreasing sweep velocity is still in line with our simple picture. For coupling strengths \( \alpha \geq 1/\sqrt{2} \) no bath influence is expected anymore [4] for the Landau-Zener probability, consistent with our data. Therefore, we focus on \( \alpha \leq 0.2 \). At the same time the excitation survival probability is expected to follow \( Q_{sc} = P_0(1 - P_0) \) at strong coupling and low temperatures [27]. As seen in Fig. 11 \( Q \) indeed approaches \( Q_{sc} \) with decreasing temperature for \( \alpha = 0.2 \).

This striking behavior of the excitation survival probability at strong coupling opens a road to determine the coupling strengths in experimental systems. Under weak coupling conditions, the minimum in the Landau-Zener probability allows to obtain \( \alpha \). For strong coupling, the minimum vanishes but the excitation survival probability still shows a clear peak. Especially the temperature dependence of the peak clearly separates strong from weak coupling. For strong coupling, the peak height increases with temperature while for weak coupling, the peak height decreases with increasing temperature.

### 4.5. Dependence of \( P \) and \( Q \) on the system-bath coupling

Next, we investigate the dependence of \( P \) and \( Q \) on the system-bath coupling in the regime of weak coupling. Fig. 12 shows the Landau-Zener probability for different \( \alpha \) at a fixed temperature \( T = 4\Delta_0 \). For increasing coupling, \( v_{\text{min}} \) shifts to larger velocities. In fact, \( v_{\text{min}} \) depends linearly on \( \alpha \), see inset of Fig. 12. The linear dependence is also predicted by our model, i.e., \( v_{\text{min}} = 15.8\alpha\Delta_0^2 \), in very good agreement with the fit \( v_{\text{min}} = 17.54\alpha\Delta_0^2 \). The decreasing maximum \( P(v_{\text{max}}) \) results from the shifting minimum. Another remarkable fact is that the Landau-Zener probability \( P(v_{\text{min}}) \) at the minimum velocity is independent of \( \alpha \), as predicted by our physical picture, see Eq. (8). We estimate the averaged splitting \( \Delta_v = T/2 = 2\Delta_0 \) in fair agreement with \( \Delta_v = 2.476\Delta_0 \), obtained with \( P(v_{\text{min}}) = \frac{1}{2}[1 + \tanh(\Delta_v/2T)] \) from the data in Fig. 12. This agreement strongly supports our physical picture that relaxation dominates in the intermediate temperature range for small sweep velocities.

The excitation survival probability \( Q \) is shown in Fig. 13 for different \( \alpha \) at a fixed temperature \( T = 4\Delta_0 \). For increasing coupling, \( v_a \) shifts to larger velocities. As before \( v_{\text{min}} \) for the Landau-Zener probability, now \( v_a \) for the excitation survival probability depends linearly on \( \alpha \), see inset of Fig. 13. Again, the linear dependence is predicted by our model, i.e., \( v_a = 3.23\alpha\Delta_0^2 \) (taking the previously determined factor \( f_a = 3.04 \) into account), in very good agreement with the fit \( v_{\text{min}} = 37.4\omega_c\Delta_0^2 \). The decreasing peak height in \( Q \) results from the shifting \( v_a \).

#### 4.6. Dependence on cut-off frequency

There is an additional time scale provided by the bath dynamics, which determines how fast the bath relaxes to its own thermal equilibrium due to the coupling to the system. It is given by the reorganization energy [29] and depends on the cut-off frequency \( \omega_c \) of the bath spectrum. In turn, the relaxation rate [29] also depends on \( \omega_c \) and relaxation is strongly suppressed when \( \Delta_v > \omega_c \). Fig. 13 shows \( P \) and Fig. 14 shows \( Q \) for different \( \omega_c \), ranging down to \( \omega_c = 0.5\Delta_v \). Such small values of the cut-off frequency describe slow bath fluctuations, a situation, for instance, typical for the biomolecular exciton dynamics in a protein-solvent environment [10]. With decreasing cut-off frequencies, the minimum in \( P(v) \) as well as \( v_a \) in \( Q \) shift to smaller \( v \) as qualitatively expected from Eq. (9) and (13) respectively. We note that this is rather surprising since a small \( \omega_c \) also induces strong non-Markovian effects. At the same time, the Landau-Zener probability \( P(v_{\text{min}}) \) decreases. With decreasing \( \omega_c \), the resonance time \( t_r \) and the averaged energy splitting \( \Delta_v \) also decrease. For cut-off frequencies \( T \leq \omega_c \), we expect \( v_{\text{min}} = 0.19\exp(-2\Delta_0/\omega_c) \), in fair agreement with the fit \( v_{\text{min}} = 0.23\exp(-2\Delta_0/\omega_c) \). This is shown in the upper inset in Fig. 13. The lower inset shows \( P(v_{\text{min}}) \) versus \( \omega_c \). The solid lines are predictions from our model and are in fair agreement with data. A similar analysis for \( v_a \) was not possible since for small \( \omega_c \) the excitation survival
probability $Q(v)$ did not sharply fall below $\frac{1}{2}$ and thus $v_a$ could not be determined unambiguously.

5. Summary

We have investigated the dissipative Landau-Zener problem by means of the numerically exact quasadiabatic propagator path-integral approach for an Ohmic bath. Thereby we discussed the Landau-Zener probability (to end up in the ground state when starting in the ground state) as well as the excitation survival probability (to end up in the excited state when starting in the excited state). In the limits of large and small sweep velocities and low temperatures, our results coincide with analytical predictions 24, 27, 25, 32. In the intermediate regime, when the sweep velocities are comparable to the minimal Landau-Zener gap and intermediate temperatures, we have identified novel non-monotonic dependencies of the Landau-Zener probabilities on the sweep velocity, temperature, system-bath coupling strength and cut-off frequency. This parameter range is clearly not accessible by perturbative means. The observed behavior can be understood in rather simple physical terms as a nontrivial competition between relaxation and Landau-Zener driving. The main difference between the Landau-Zener and the excitation survival probability results from the simple fact that the excited state can always decay via spontaneous emission while the ground state needs a thermally excited phonon in order to become excited. Thus even at vanishing temperature the excitation survival probability decreases strongly for small enough driving speed whereas the Landau-Zener probability only for high temperatures. As nowadays advanced experimental set-ups allow for a rather comprehensive control of the parameters, this novel feature should be accessible by available experimental techniques.

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Figure 1: The spectrum of a two-level system driven linearly in time through an avoided crossing. The solid lines mark the exact energies whereas the dashed lines give the crossing energies $\pm vt$ of the diabatic states. In addition, the resonance time window of width $t_r$ around $t = 0$ is shown, in which $\Delta t \leq \Delta_c$, see Sec. 4.2 for more details.

Figure 2: The occupation probability $P(t)$ of the diabatic state $|\uparrow\rangle$ versus time and temperature is shown for a slow sweep velocity $v = 0.02\Delta_0^2$, a weak system bath coupling $\alpha = 0.0016$ and a large cut-off frequency $\omega_c = 10\Delta_0$. The time is restricted around the crossover which was at $t_{\text{cross}} = 2500/\Delta_0$.

Figure 3: The time derivative $dP/dt$ corresponding to Fig. 2.

Figure 4: The Landau-Zener probability $P$ for various temperatures $T$ is shown for a weak system-bath coupling $\alpha = 0.0016$. The dotted lines are guides to the eye. The solid line marks the coherent Landau-Zener probability $P_0$, while the dot-dashed line indicates the high-temperature limit $P_{\text{SD}}$, see text.
Figure 5: Comparison of the Landau-Zener ($P$, top panel, triangles) and the excitation survival ($Q$, bottom panel, circles) probability with perturbative approaches for $T = 4\Delta_0$ for a weak system-bath coupling $\alpha = 0.0016$. The thick solid line in both panels marks the standard Landau-Zener probability $P_0$, while the dot-dashed line shows $P_{SD}$. The dotted lines show the behavior according to Ao and Rammer [24], the dashed lines according to Kayanuma and Nakayama [27]. Moreover, in the top panel, the dash-dash-dotted line marks the result of Pokrovsky and Sun [28] (which only give a formula for the Landau-Zener probability $P$). In the lower panel, the dot-dot-dashed line indicates $P_0(1 - P_0)$.

Figure 6: Main: Landau-Zener probability $P(v = 0.005\Delta_0^2)$ at the smallest sweep velocity (blue diamonds), $P_c$ of Eq. (6) (blue solid line), Landau-Zener probability $P(v_{\text{min}})$ at the sweep velocity of the minimum (black circles), and $P_{\text{min}}$ of Eq. (8) (black solid line) versus temperature. Inset: The minimum sweep velocity (red squares) extracted from the data of Fig. 4 and $v_{\text{min}}$ according to Eq. (10) (red dotted line). The coupling strength is $\alpha = 0.0016$.

Figure 7: The excitation survival probability $Q$ for various temperatures $T$ is shown for a weak system-bath coupling $\alpha = 0.0016$. The dotted lines are guides to the eye. The solid line marks the coherent excitation survival probability $Q_0 = P_0$ which is identical to the Landau-Zener probability. The dot-dashed line indicates the high-temperature limit $P_{\text{SD}}$ and the dot-dot-dashed line indicates the strong coupling limit $Q_{sc} = P_0(1 - P_0)$.

Figure 8: Main: Sweep velocity $v_a = v[Q(T) = \frac{1}{2}\Delta_0]$ (with temperature fixed) for which the resonance time (Eq. (5)) coincides with the relaxation time (up to a prefactor $f_a$) vs. temperature. Inset: Critical excitation survival probability $Q_c$, Eq. (14) (solid line), and $Q(v = 0.005\Delta_0^2)$ extracted from Fig. 4 versus temperature for $\alpha = 0.0016$. 

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Figure 9: The Landau-Zener probability $P$ for various temperatures $T$ is shown for an intermediate value of the system-bath coupling $\alpha = 0.02$. The dotted lines are guides to the eye. The solid line marks the coherent Landau-Zener probability $P_0$, while the dot-dashed line indicates the high-temperature limit $P_{SD}$.

Figure 10: The excitation survival probability $Q$ corresponding to the case shown in Fig. 9. Here, the dot-dot-dashed line marks the strong coupling limit $Q_{sc} = P_0(1 - P_0)$.

Figure 11: The Landau-Zener ($P$, all data above the red dash-dotted line) and the excitation survival ($Q$, all data below the red dash-dotted line) probability for various temperatures $T$ are shown for strong system-bath coupling $\alpha = 0.2$. The dotted lines are guides to the eye. The solid line marks the coherent excitation probability which is identical to the coherent Landau-Zener probability $P_0$.

Figure 12: Landau-Zener probability $P$ for different $\alpha$ for $T = 4\Delta_0$. Inset: Linear dependence of $v_{\min}$ on $\alpha$, see text.
Figure 13: Excitation survival probability $Q$ for different $\alpha$ for $T = 4\Delta_0$. Inset: Linear dependence of $v_a$ on $\alpha$, see text.

Figure 14: Landau-Zener probability $P$ for various cut-off frequencies $\omega_c$ for $T = 4\Delta_0$ and $\alpha = 0.00985$. Insets: $P(v_{\min})$ (bottom) and $v_{\min}$ (top) vs $\omega_c$; solid lines: model predictions, see text.

Figure 15: Excitation survival probability $Q$ corresponding to Fig. 14.