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Davydov-Ansatz for Landau-Zener-Stueckelberg-Majorana transitions in an environment: Tuning the survival probability via number state excitation

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ABSTRACT

We theoretically investigate transitions in a two-level system, which are induced by a sweep through an avoided crossing in the presence of coupling to a single, excited bosonic mode. This allows us to propose an initial number-state bosonic excitation as a new possible control parameter for the survival probability at long times. The expansion of number states in terms of coherent states centered around points on a circle in phase space makes a multi-Davydov-Ansatz the method of choice to perform the required numerical calculations. It is revealed that the starting time of the transition greatly affects the final transition probabilities. In addition, we found that the mixing angle, which is tuning between the diagonal and off-diagonal coupling, is decisive for the ability to control the transition via number state excitation. For a mixing angle of $\pi/4$, we found the maximal effect of number state excitation on the transition probability.

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I. INTRODUCTION

In the course of a Landau-Zener (LZ) transition, energy levels of a two-level system undergo an avoided crossing under an action of the external drive.^{1,2} This celebrated physical phenomenon was independently studied by Landau, Zener, Stueckelberg, and Majorana in 1932, and the standard LZ model is also referred to as the Landau-Zener-Stueckelberg-Majorana (LZSM) model,^{1–4} which has found applications in a broad range of fields, including atomic and molecular physics,^{5–10} quantum optics,¹¹ solid state physics,¹² chemical physics,^{13,14} and quantum information science.¹⁵ Recently, the LZSM model has received renewed interest as the number of physical systems described by the LZSM model grows. New applications of the LZSM model have been

reported in a nitrogen-vacancy center in a diamond lattice,¹⁵ a one-electron semiconductor double quantum dot,¹⁶ and an accelerated Bose-Einstein condensate that is synthetically spin-orbit coupled.¹⁷

Particularly interesting applications of the LZSM model are the devices in circuit quantum electrodynamics (QED).^{18–21} In 2004, Wallraff *et al.* performed an experiment in which a charge qubit is coupled to a superconducting transmission line resonator,²² and Chiorescu *et al.* fabricated a superconducting flux qubit coupled to a quantum interference device.²³ Such QED configurations are the solid-state analog of a two-level atom. Parameters in the superconducting circuits can be tuned over a wide range, allowing for efficient control of the qubits and transmission line resonators. For example, Astafiev *et al.* built an artificial-atom maser consisting of a

resonator and a Josephson-junction charge qubit coupled to it. The charge qubit is made of a superconducting Al island connected to a ground through two Josephson junctions with superconducting quantum interference device (SQUID) geometry so that the effective Josephson energy is controlled by the magnetic flux through the loop.²⁴

In 2004, the LZSM mechanism was observed by Izmalkov *et al.* in an Al three-junction qubit coupled to a Nb resonant tank circuit, and output signals were found to depend on surrounding environments.²⁵ Environmental effects on the QED device can be modeled by coupling a set of harmonic oscillators to the LZSM model.²⁶ In the framework of the dissipative LZSM model, final transition probabilities in the fast and slow sweeping limit have been studied in 1989 using time-dependent perturbation theory.²⁷ Inspired by the realization of LZSM physics in QED devices, Hänggi and co-workers systematically investigated the final transition probabilities influenced by the bosonic bath at zero temperature.^{26,28} Nalbach *et al.* studied extensively thermal effects in the dissipative LZSM model using the quasi-adiabatic propagator path integral method and the nonequilibrium Bloch equations.^{29–33} A random-variable driving approach pioneered in Refs. 34 and 35 has been used by Stockburger³⁶ as well as by Orth *et al.*^{37,38} in the present context. Furthermore, Sun *et al.* applied the hierarchy equation method³⁹ to the dissipative LZSM model. Recently, Huang and Zhao adopted the multiple Davydov trial states to elucidate the dissipative LZSM dynamics.⁴⁰

While much is still unknown about the underlying physics of the dissipative LZSM model, recent attention has been devoted to a superconducting qubit coupled to a single harmonic oscillator of frequency ω .^{18,24,40–43} For example, a circuit QED device has been experimentally realized by coupling the charge qubit to the superconducting resonator through an electric field. The charge qubit and the resonator have been used to represent the standard LZSM model and the harmonic oscillator, respectively.²⁴ Saito *et al.* have revealed in their model that the dynamics at zero temperature depends strongly on the oscillator frequency only at intermediate times, if the oscillator is in its ground state at $t \rightarrow -\infty$.¹⁸ Sun *et al.* compared the dynamics with rotating-wave approximation (RWA) and without RWA when the initial state of the oscillator is assumed to be a superposition of coherent states, implying that the RWA method is inaccurate for this problem. Ashhab considered the final probabilities when the harmonic oscillator mode is initially set to a finite-temperature thermal equilibrium state. Huang and Zhao found two-stage LZ transitions induced by the combined effect of tunneling strength Δ and the off-diagonal qubit-oscillator coupling.⁴⁰ In 2018, Malla *et al.* aimed to find the analytical solution of slow and fast oscillators ($\omega < \Delta$ and $\omega > \Delta$, where ω is the frequency of the harmonic oscillator) when there are many quanta excited initially. Although many efforts have been devoted to understanding the LZSM model, there exist several unsettled fundamental issues: the influence on LZ transitions of an initially excited environment as well as the effect of different oscillator frequencies in the intermediate regime ($\omega \sim \Delta$) on the final probability. Moreover, the off-diagonal qubit-oscillator coupling has not been adequately treated if the initial oscillator state is not the vacuum state.^{41–43} In this work, we will shed some light on the issues mentioned by investigating how an initial number state of the oscillator affects the LZSM dynamics of a two-level system coupled to a single harmonic

oscillator using the multi- D_2 -Ansatz with the Dirac-Frenkel variational principle.

The remainder of the paper is structured as follows. In Sec. II, we present the model Hamiltonian and we give our trial wave function, the multi- D_2 -Ansatz, in Sec. III. The effect of initial number state excitation on the final transition probability is numerically examined in Sec. IV. Conclusions drawn are in Sec. V. Some properties of displaced number states and the (generalized) Laguerre polynomials are gathered in the Appendix.

II. LZSM MODEL IN THE PRESENCE OF A BOSONIC MODE

The Hamiltonian for transitions in the dynamics of a single spin 1/2 coupled to a single harmonic degree of freedom is given by

$$\hat{H} = \frac{\varepsilon(t)}{2} \hat{\sigma}_z + \frac{\Delta}{2} \hat{\sigma}_x + \omega \hat{a}^\dagger \hat{a} + \frac{\lambda}{2} (\cos \theta \hat{\sigma}_z + \sin \theta \hat{\sigma}_x) (\hat{a}^\dagger + \hat{a}), \quad (1)$$

with Pauli spin matrices $\hat{\sigma}_x$ and $\hat{\sigma}_z$, time-dependent asymmetry parameter $\varepsilon(t) = vt$ with sweeping velocity v , tunneling splitting Δ , and two coupling strengths

$$\lambda_z = \lambda \cos \theta, \quad \lambda_x = \lambda \sin \theta, \quad (2)$$

where a change in the mixing angle θ allows us to switch between the diagonal ($\theta = 0$) and off-diagonal coupling ($\theta = \pi/2$). Here, $\hbar$ is set to unity and the zero point energy of the oscillator has been omitted. Without coupling to the (single) oscillator, the standard LZSM model Hamiltonian has been studied by Landau,¹ as well as by Zener,² Stueckelberg,³ and Majorana.⁴ With coupling to the bosonic mode, the above model is related to the celebrated quantum Rabi-model,⁴⁴ in which case the asymmetry parameter is time-independent. In the semi-classical Rabi-model, the bosonic mode is replaced by a sinusoidal driving field that is not influenced by the spin degree of freedom.⁴⁵

For large negative times, the term proportional to σ_z dominates the Hamiltonian. Let us, therefore, introduce the so-called diabatic system basis $|\pm\rangle$, which are the eigenstates of $\hat{\sigma}_z$, i.e., of $\hat{H}_{\text{LZ}} = \frac{\varepsilon(t)}{2} \hat{\sigma}_z + \frac{\Delta}{2} \hat{\sigma}_x$ for $|t| \rightarrow \pm\infty$. Furthermore, we denote by $|n\rangle$ the eigenstates of the bare environmental Hamiltonian $\hat{H}_{\text{env}} = \omega \hat{a}^\dagger \hat{a}$. Due to the coupling to the spin, the oscillator eigenstates in the subspace of the projected Hamiltonian corresponding to spin up and spin down states are changed to

$$|n_\pm\rangle = \hat{D}[\mp C]|n\rangle, \quad C = \frac{\lambda \cos \theta}{2\omega}, \quad (3)$$

respectively, as can be shown by a completion of the square argument.¹⁸ Here, the displacement operator

$$\hat{D}[C] = \exp[C\hat{a}^\dagger - C^*\hat{a}] \quad (4)$$

has been used, whose properties are gathered in the Appendix.

In the presence of environmental coupling, the analytical result for the probability to remain in the initial state if the system is

initially (i.e., for $t \rightarrow -\infty$) in the diabatic ground state $|0_+\rangle|+\rangle$ is given by¹⁸

$$p(t \rightarrow \infty) = \exp \left[\frac{-\pi \left(\left(\Delta - \frac{\lambda^2}{2\omega} \sin(2\theta) \right)^2 + \lambda^2 \sin^2 \theta \right)}{2|v|} \right]. \quad (5)$$

One can read off from this result that, even in the presence of coupling to the oscillator, the asymptotic result for the staying probability is unaffected, leading to the celebrated Landau-Zener result

$$p(t \rightarrow \infty) = \exp \left[\frac{-\pi |\Delta|^2}{2|v|} \right], \quad (6)$$

if the coupling is purely longitudinal ($\theta = 0$).^{26,28} Furthermore, in combination with the no-go-theorem of Saito,²⁸ one can read off from (5) the probability $P(t) = |\langle \Psi(t) | - \rangle|^2$ for the system to be in the diabatic down state if initially $|\Psi(t=0)\rangle = |0_+\rangle|+\rangle$, for $t \rightarrow \infty$,

$$\begin{aligned} P(t \rightarrow \infty) &= 1 - p(t \rightarrow \infty) \\ &= 1 - \exp \left[\frac{-\pi \left(\left(\Delta - \frac{\lambda^2}{2\omega} \sin(2\theta) \right)^2 + \lambda^2 \sin^2 \theta \right)}{2|v|} \right]. \end{aligned} \quad (7)$$

The general formula allows for a tuning of the steady state survival probability via several different strategies. Apart from the most obvious ones of changing the tunneling splitting and/or the sweep velocity, which are suggested by the Landau-Zener formula, another one would be to change the mixing angle θ between the diagonal and off-diagonal coupling⁴⁰ and/or the coupling strength. We note in passing that, for $\theta = 0$, a change in the oscillator frequency does not affect the asymptotic result if started from the ground state. For initially highly excited (number) states, the oscillator frequency does play a role for the steady state result, however.⁴³

Number states can be generated experimentally in cavities as has been shown by Haroche and co-workers. In 2007, his group fabricated an open cavity made up of two superconducting niobium mirrors facing each other and detected the birth of a photon in a cavity.⁴⁶ In detail, a small coherent field was produced after a microwave pulse was radiated by a classical source and scattered on the edges of the cavity mirrors. The field was then injected inside the cavity, leading to the creation of a superposition of photon number states.⁴⁷ Still another option, therefore, would be to change the initial excitation of the boson. This last possibility to control the steady state probability is in the focus of interest of the theoretical studies in the present manuscript.

III. DAVYDOV-ANSATZ

In the following, we will consider two different approaches to the dynamics starting from the $|+\rangle$ state of the spin and with an initial excitation into a displaced eigenstate of the bath degree of

freedom (a displaced number state); that is, we assume the initial wavefunction to be

$$|\Psi(t=0)\rangle = |+\rangle \hat{D}^\dagger[C]|n\rangle. \quad (8)$$

In a first approach, we will derive relatively complex equations of motion that depend on the initial excitation state index but have trivial initial conditions. Second, we will expand the initially excited oscillator state in terms of coherent states, leading to more standard equations but with nontrivial initial conditions that have to be sampled along a circle in phase space. In both cases, we will use a multi-Davydov-Ansatz of D_2 complexity.

The original Davydov-Ansatz led to the prediction of solitonic excitations in proteins, proposed in the 1970s by Davydov and co-workers.^{48–51} The stability of those excitations at finite temperature has been intensively debated in the 1980s and 1990s.^{52,53} More recently, Zhao and co-workers have successfully applied various versions of Davydov-Ansatz for the investigation of spin-boson problems^{54,55} and Holstein molecular-crystal models.^{56–59}

Since a simple Davydov-Ansatz can, in general, only account for an approximate solution of the time-dependent Schrödinger equation, multiple Davydov-Ansatz types⁵⁸ have been recently proposed and used. These in principle allow for an exact solution of the time-dependent Schrödinger equation. A recent comparison of different variants of the Davydov-Ansatz is given in Ref. 60. The multi- D_2 -Ansatz

$$|\Psi_{D_2}^M(t)\rangle = \sum_{k=1}^M (A_k(t)|+\rangle \hat{D}[f_k(t)]|0\rangle + B_k(t)|-\rangle \hat{D}[f_k(t)]|0\rangle) \quad (9)$$

for the oscillator starting in its ground state is commonly viewed as a special case of the multi- D_1 -Ansatz

$$|\Psi_{D_1}^M(t)\rangle = \sum_{k=1}^M (A_k(t)|+\rangle \hat{D}[f_k(t)]|0\rangle + B_k(t)|-\rangle \hat{D}[g_k(t)]|0\rangle). \quad (10)$$

We outline briefly why it is advantageous, however, to employ the multi- D_2 -Ansatz rather than the multi- D_1 -Ansatz in the LZSM model. This is because, in contrast to the standard quantum Rabi model, the LZSM model does not exhibit a natural fixed system basis, due to the time-dependence of the asymmetry parameter. But while the multi- D_1 -Ansatz singles out elements of the system basis $\{|+\rangle, |-\rangle\}$, the multi- D_2 -Ansatz

$$|\Psi_{D_2}^M(t)\rangle = \sum_{k=1}^M (A_k(t)|+\rangle + B_k(t)|-\rangle) \hat{D}[f_k(t)]|0\rangle \quad (11)$$

does not. In this form, the D_1 -Ansatz indeed appears as a special case of the D_2 -Ansatz: $A_k(t) = 0$ for even k and $B_k(t) = 0$ for odd k . This theoretical consideration is confirmed by our numerical calculations, which show that it is much harder to converge the D_1 -Ansatz to the exact result than the D_2 -Ansatz.

A. Excitation dependent equations of motion

The multi- D_2 -Ansatz with multiplicity M for displaced number states, i.e., number states in the bath degree of freedom that are acted

on by the displacement operator, is given by

$$|\Psi_{D_2,n}^M(t)\rangle = \sum_{k=1}^M \left(A_k(t)|+\rangle + B_k(t)|-\rangle \right) \hat{D}[f_k(t)]|n\rangle, \quad (12)$$

and we suppress the index n from now on. Especially for $n = 0$, the action of the displacement operator [defined in (4)] on the ground state $|n = 0\rangle$ of the harmonic oscillator creates a coherent state

$$|\alpha\rangle := \hat{D}[\alpha]|0\rangle. \quad (13)$$

The action of this operator on number states leads to displaced number states, which were studied in detail by Nieto.⁶¹ Like the simple coherent states, displaced number states form an overcomplete set of states for fixed n ⁶²

$$\frac{1}{\pi} \int d^2\alpha \hat{D}[\alpha]|n\rangle\langle n|\hat{D}^\dagger[\alpha] = 1. \quad (14)$$

This ensures the convergence of the Ansatz (12) if the multiplicity M is large enough. The equations of motion of the time-dependent parameters $\tilde{u} = \{A_j(t), B_j(t), f_j(t)\}$ can be derived from the Dirac-Frenkel variational principle in its Lagrangian form.^{63–66} The Davydov Dirac-Frenkel Lagrangian reads (for normalized trial

wavefunctions, the derivative may act only to the right, simplifying matters considerably)

$$L_{D_2} = \left\langle \Psi_{D_2}^M(t) \left| \left(i \frac{\partial}{\partial t} - \hat{H} \right) \right| \Psi_{D_2}^M(t) \right\rangle =: L_{\text{td}} - L_H. \quad (15)$$

Using the orthogonality of the spin states, the time derivative (A13) of the displacement operator, and the overlap of displaced number states (A14) from the Appendix, we get

$$L_{\text{td}} = i \sum_{j,k} \left\{ \left[A_k^* \dot{A}_j + B_k^* \dot{B}_j - (A_k^* A_j + B_k^* B_j) \frac{\dot{f}_j(f_j^* - 2f_k^*) + f_j \dot{f}_j^*}{2} \right] \right. \\ \times L_n(|f_j - f_k|^2) - (A_k^* A_j + B_k^* B_j) [\dot{f}_j(f_j - f_k)^* \\ \left. + \dot{f}_j^*(f_j - f_k)] L_{n-1}^{(1)}(|f_j - f_k|^2) \right\} S_{kj} \quad (16)$$

for the time derivative part of the Lagrangian, where

$$S_{kj} = \langle 0 | \hat{D}^\dagger[f_k] \hat{D}[f_j] | 0 \rangle = e^{-(|f_k|^2 + |f_j|^2)/2 + f_k^* f_j} \quad (17)$$

is the overlap between two coherent states, and where the Laguerre polynomials $L_n(x)$ and the associated Laguerre polynomials discussed in the Appendix have been used. Furthermore,

$$L_H = \sum_{j,k} \left\{ \left[\frac{\varepsilon(t)}{2} (A_k^* A_j - B_k^* B_j) + \frac{\Delta}{2} (A_k^* B_j + B_k^* A_j) \right] L_n(|f_j - f_k|^2) + \omega (A_k^* A_j + B_k^* B_j) [f_k^* f_j L_n(|f_j - f_k|^2) + n L_{n-1}(|f_j - f_k|^2) \right. \right. \\ \left. \left. - [f_j(f_j - f_k)^* - f_k^*(f_j - f_k)] L_{n-1}^{(1)}(|f_j - f_k|^2) \right] + \left[\frac{\lambda_z}{2} (A_k^* A_j - B_k^* B_j) + \frac{\lambda_x}{2} (A_k^* B_j + B_k^* A_j) \right] \right. \\ \left. \times [(f_k^* + f_j) L_n(|f_j - f_k|^2) - [(f_j - f_k)^* - (f_j - f_k)] L_{n-1}^{(1)}(|f_j - f_k|^2)] \right\} S_{kj} \quad (18)$$

is found for the Hamiltonian part of the Lagrangian.

The Eulerian equations of motion,

$$\frac{d}{dt} \frac{\partial L_D}{\partial \dot{u}_i^*} - \frac{\partial L_D}{\partial u_i^*} = 0, \quad (19)$$

are (with the argument $|f_j - f_k|^2$ of the Laguerre polynomials suppressed)

$$i \sum_j \left\{ \left(\dot{A}_j - A_j \frac{\dot{f}_j(f_j^* - 2f_k^*) + f_j \dot{f}_j^*}{2} \right) L_n - A_j [\dot{f}_j(f_j - f_k)^* + \dot{f}_j^*(f_j - f_k)] L_{n-1}^{(1)} \right\} S_{kj} \\ = \sum_j \left\{ \left(\frac{v t}{2} A_j + \frac{\Delta}{2} B_j \right) L_n + \omega A_j \{ f_k^* f_j L_n + n L_{n-1} - [f_j(f_j - f_k)^* - f_k^*(f_j - f_k)] L_{n-1}^{(1)} \} \right. \\ \left. + \left[\frac{\lambda_z}{2} A_j + \frac{\lambda_x}{2} B_j \right] \{ (f_k^* + f_j) L_n - [(f_j - f_k)^* - (f_j - f_k)] L_{n-1}^{(1)} \} \right\} S_{kj} \quad (20)$$

and a similar equation for B_j with sign changes in front of the terms proportional to vt as well as to λ_z .

Furthermore, the equation of motion for the coherent state parameter is

$$\begin{aligned}
& i \sum_j \left\{ \left[A_k^* A_j + B_k^* B_j - (A_k^* A_j + B_k^* B_j) \frac{f_j^* \dot{f}_j + f_j \dot{f}_j^*}{2} \right] (f_j L_n + (f_j - f_k) L_{n-1}^1) + (A_k^* A_j + B_k^* B_j) \dot{f}_j \right. \\
& \quad \times \left[(1 + f_k^* f_j) L_n + (f_k^* (f_j - f_k) + f_j (f_k - f_j)^*) L_{n-1}^1 + n L_{n-1} \right] - (A_k^* A_j + B_k^* B_j) \dot{f}_j^* \left[f_k (f_j - f_k) L_{n-1}^1 + (f_j - f_k)^2 L_{n-2}^2 \right] \Big\} S_{kj} \\
& = \sum_j \left\{ \left[\frac{v t}{2} (A_k^* A_j - B_k^* B_j) + \frac{\Delta}{2} (A_k^* B_j + B_k^* A_j) \right] (f_j L_n + (f_j - f_k) L_{n-1}^1) + \omega (A_k^* A_j + B_k^* B_j) \right. \\
& \quad \times \left[f_j (|f_k|^2 + n + 1) L_n + ((f_j - f_k) (|f_k|^2 + n + 1) + f_k f_j (f_k - f_j)^*) L_{n-1}^1 + n f_k L_{n-1} + f_k^* (f_j - f_k)^2 L_{n-2}^2 + f_k^* f_j (f_j - f_k) L_n^1 \right] \\
& \quad \left. + \left(\frac{\lambda_z}{2} (A_k^* A_j - B_k^* B_j) + \frac{\lambda_x}{2} (A_k^* B_j + B_k^* A_j) \right) \right] \left[(1 + f_k^* f_j + f_j^2) L_n + ((f_k^* + f_j + f_k) (f_j - f_k) + f_j (f_k - f_j)^*) L_{n-1}^1 + n L_{n-1} + (f_j - f_k)^2 L_{n-2}^2 \right] \Big\} S_{kj},
\end{aligned} \quad (21)$$

where (20) and its complex conjugate help to simplify the result.⁶⁷ The initial conditions for the coefficients of the spin states are $A_1 = 1$, $B_1 = 0$ and $A_k = B_k = 0$, $\forall k \neq 1$. Furthermore, $f_1 = -C$, as can be seen from the Ansatz, and all other initial displacements are arbitrary. The equations above are quite complex with simple initial conditions. Below, we are therefore presenting a second approach which is based on simpler equations but with different (more complex) initial conditions.

B. Expansion of the environmental excitation in terms of coherent states

As laid out in Refs. 68 and 69, we may write a number state $|n\rangle$ of the harmonic oscillator as

$$|n\rangle = \frac{1}{2\pi} \sqrt{\frac{n! e^{|\beta|^2}}{|\beta|^{2n}}} \int_{-\pi}^{\pi} d\theta e^{-in\theta} |\beta| e^{i\theta}. \quad (22)$$

This is a one-dimensional integral along a circle in phase space, in contrast to what one would get if the straightforward decomposition of the unit operator in terms of coherent states (14) was used. Then, one would end up with a two-dimensional integral over phase space and a much less user-friendly numerical scheme would result (because for the calculation of expectation values, two decompositions of unity and in fact a four-dimensional integral would be needed). The fact that a single integral is sufficient is deeply rooted in the overcompleteness of the coherent states.⁶⁹

For a numerical treatment, we have to transform the integral into a sum. In order to discretize the integral over θ , we fix $N \in \mathbb{N}$ and set

$$\theta_k := -\pi + \frac{2\pi}{N} k, \quad k = 0, \dots, N-1. \quad (23)$$

Thus,

$$|n\rangle \approx \sqrt{\frac{n! e^{|\beta|^2}}{|\beta|^{2n}}} \frac{1}{N} \sum_{k=0}^{N-1} e^{-in\theta_k} |\beta| e^{i\theta_k}. \quad (24)$$

In his book,⁶⁹ Schleich mentions that β , although arbitrary in principle, should be chosen such that $|\beta| = \sqrt{n}$.

The multi-D₂-Ansatz with multiplicity M for the propagation of one of the coherent states $|\beta| e^{i\theta_k}$ above reads

$$|\Psi_{D_2}^M(k, t)\rangle = \sum_{m=1}^M \sum_{j=\pm} A_{kjm}(t) |f_{km}(t)\rangle |j\rangle, \quad (25)$$

where $|\pm\rangle$ are the eigenstates of σ_z and $|f_{km}(t)\rangle$ are coherent states. In contrast to the presentation above, we have now a triply indexed quantity $A_{kjm}(t)$. This is due to the fact that we are using only one symbol for the two coefficients A and B , where the former A is now A_{kjm} (with middle index $+$) and the former B is A_{kjm} (with middle index $-$). Furthermore, the index with respect to the discretization of the angular integration in the representation of the number state is the new first index k . The equations of motion are the ones from above but with $n = 0$ leading to a dramatic simplification because the Laguerre polynomial with index zero is one (see the Appendix) and all the associated Laguerre polynomials are zero apart from L_n^1 .

The initial conditions read

$$A_{kjm}(0) = \begin{cases} 1, & j = +, m = 1, \\ 0, & \text{else,} \end{cases} \quad f_{km}(0) = \begin{cases} |\beta| e^{i\theta_k}, & m = 1, \\ 0, & \text{else.} \end{cases} \quad (26)$$

The full wavefunction is then approximated by

$$|\Psi_{D_2}^M(t)\rangle \approx \sqrt{\frac{n! e^{|\beta|^2}}{|\beta|^{2n}}} \frac{1}{N} \sum_{k=0}^N e^{-in\theta_k} |\Psi_{D_2}^M(k, t)\rangle, \quad (27)$$

which contains a double sum, i.e., a sum over multiplicity as well as over the discretization index.

For large N , this becomes numerically demanding. Let us thus have a look at a slightly different approach in terms of a single sum (apart from the trivial sum over $\pm$). The multi-D₂-Ansatz with multiplicity $M \geq N$ for the propagation of the full expression (24) reads

$$|\Psi_{D_2}^M(t)\rangle = \sum_{m=1}^M \sum_{j=\pm} A'_{jm}(t) |f_m(t)\rangle |j\rangle, \quad (28)$$

with just two indices for the A' coefficients. The initial conditions then read

$$A'_{jm}(0) = \begin{cases} \mathcal{N}(\beta) e^{-in\theta_m}, & m < N, j = +, \\ 0, & \text{else,} \end{cases} \quad f_m(0) = \begin{cases} |\beta| e^{i\theta_m}, & m < N, \\ \text{arb.}, & \text{else,} \end{cases} \quad (29)$$

and are displayed in Fig. 1. The normalization constant is

$$\mathcal{N}(\beta) = \sqrt{\frac{n! e^{|\beta|^2}}{|\beta|^{2n}}} \frac{1}{N}. \quad (30)$$

The positions of the arbitrary displacements have to follow two constraints. First, they should not be too close, in order to avoid singularities, when making the equations explicit, and second, they should also be not too far apart because otherwise the representation of unity will not be good enough. More details regarding the second point can be found in Ref. 70.

In order to propagate the diabatic states $|n_+\rangle|+\rangle = \hat{D}[-C]|n\rangle|+\rangle$, one has to include the action of $\hat{D}[-C]$ in the sum (28). To this end, one may use the fact that each coherent state in the Davydov-Ansatz can be viewed as a displacement-operator acting on the ground state

$$\hat{D}[-C]|\alpha\rangle = \hat{D}[-C]\hat{D}[\alpha]|0\rangle = \exp\left[-\frac{C}{2}(\alpha - \alpha^*)\right] \hat{D}[\alpha - C]|0\rangle. \quad (31)$$

The inclusion of the action of $\hat{D}[-C]$ on the sum (28) thus can be done by multiplying the initial values of the coefficients by the prefactor $\exp\left[-\frac{C}{2}(\alpha - \alpha^*)\right]$ and by changing the initial displacements to $f_k - C$. The expectation-value $\langle\hat{\sigma}_z\rangle$ then becomes

FIG. 1. Initial conditions in phase space if the bath excitation is expanded in terms of $N = 15$ coherent states: The blue asterisks denote the coherent states with initial conditions that are nonzero. The red asterisks denote coherent state initial conditions that come in due to nontrivial multiplicity, leading to $M = 20$, and whose corresponding expansion coefficients are initially zero.

$$\langle\hat{\sigma}_z\rangle = \langle\Psi_{D_2}^M(t)|\hat{\sigma}_z|\Psi_{D_2}^M(t)\rangle = \sum_{k,m=1}^M \sum_{j=\pm} j A_{jk}^* A_{jm} \langle f_{jk}|f_{jm}\rangle. \quad (32)$$

From this, one can derive

$$P(t) = \frac{1}{2}(1 - \langle\hat{\sigma}_z\rangle) \quad (33)$$

for the transition probability.

IV. NUMERICAL RESULTS

The parameter space of the LZSM model with coupling to a single harmonic mode is already quite large. Because we are interested in the initial state dependence of the survival probability, we first keep fixed the tunneling as well as the sweep parameter in the slow oscillator regime

$$\Delta = 1, v = \frac{\pi\Delta^2}{4}, \omega = \frac{\Delta}{4}, \quad (34)$$

and only to the very end, we also change the frequency of the oscillator.

A. Initial time dependence of transition probabilities from initial ground state

We first investigate the case $n = 0$, for which we may compare the numerical results with the analytical transition probability given by (7). The procedure described in Sec. III B can be applied one to one if we set $n = 0$, $N = 1$, $\beta = 0$, and $|\beta|^{2n} = 1$. Multiplicity M is increased until convergence is reached. First, we find from Figs. 2–4 for the three mixing angles, $\theta = 0$, $\pi/4$, and $\pi/2$, that the final transition probability depends critically on the requirement that the starting time t_0 of the propagation is sufficiently early, i.e., $t_0 \ll 0$. This can be understood from the fact that (5) is valid only if the system starts out in its ground state $\hat{D}^\dagger[C]|0\rangle|+\rangle$ at $t_0 \rightarrow -\infty$ [see Eq. (3)]. If t_0 is too close to $t = 0$, this state is not the system's ground state, and the dynamics will depend essentially on the precise value

FIG. 2. Convergence test with respect to initial time t_0 : transition probability $P(t)$ for initial excitation $n = 0$ and mixing angle $\theta = 0$, $\lambda = \Delta$, and $M = 15$. The dashed line is the analytical result. Two different starting times are indicated by colors (red: $t_0 = -5$ and blue: $t_0 = -15$). Starting time $t_0 = -15$ leads to converged outcome.

FIG. 3. Convergence test with respect to initial time t_0 : transition probability $P(t)$ for initial excitation $n = 0$ and mixing angle $\theta = \pi/4$, as well as $\lambda = \Delta$ and $M = 25$. Three different starting times are indicated by colors (red: $t_0 = -15$, green: $t_0 = -45$, and blue: $t_0 = -55$). The dashed line is the analytical result.

of t_0 . We find second that the value of $|t_0|$ which results in the correct transition probability depends on the mixing angle θ , and the largest value was found for $\theta = \pi/4$. This again follows from the same reasoning since the off-diagonal coupling transfers the diabatic states to the adiabatic ones.

B. Excited initial states

The initial times found from Figs. 2–4 are also the appropriate times to start from for higher excited states $|n\rangle$, $n > 0$. We choose $n \in [1, 50]$ for the initial excitation and a coupling strength which is renormalized by the initial excitation

$$\lambda = \frac{\Delta}{\sqrt{n}}, \quad (35)$$

FIG. 4. Convergence test with respect to initial time t_0 : transition probability $P(t)$ for initial excitation $n = 0$ and mixing angle $\theta = \pi/2$, as well as $\lambda = \Delta$ and $M = 23$. Three different starting times are indicated by colors (red: $t_0 = -10$, green: $t_0 = -15$, and blue: $t_0 = -25$). The dashed line is the analytical result.

FIG. 5. Convergence test with respect to multiplicity M : $P(t)$ for $n = 1$, $\theta = \pi/4$, and $N = 5$. $M = 20$ (blue), $M = 25$ (red), and $M = 30$ (green).

as given in Ref. 43. In Fig. 5, we show that the convergence with respect to the number N of sampling points on the circle of radius $\beta = \sqrt{n}$ is quite quick, while convergence with respect to multiplicity M occurs only slowly. Next, we choose different radii $|\beta|$ of the circle of integration, in order to examine the emphasis on the special radius $|\beta| = \sqrt{n}$ given in Ref. 69. In Fig. 6, it is shown that indeed the deviation from the special radius leads to strong deterioration of the results.

The main finding of the present work is that the initial oscillator excitation can be used as a control parameter to tune the steady value of the staying probability if the coupling is scaled according to $\lambda = \frac{\Delta}{\sqrt{n}}$ and the mixing angle $\theta \neq 0$. This is shown in Fig. 7, where a monotonic decrease in the steady state value for increasing excitation can be observed for $n > 3$. Multiplicities up to $M = 25$ have been used to obtain converged results. In Ref. 43, an (approximate) analytical reasoning for convergence of $P(t \rightarrow \infty)$ as $n \rightarrow \infty$ is given for $\theta = 0$, in conjunction with the corresponding steady state value. Although generalization of the result therein to $\theta \neq 0$ is not straightforward, our numerical calculations show that also for

FIG. 6. Convergence test with respect to β : $P(t)$ for $n = 4$, $\theta = \pi/4$, $N = 14$, and $M = 18$. $\beta = 1$ (red), $\beta = 4$ (green), and $\beta = \sqrt{n} = 2$ (blue) (in coincidence with the exact result).

FIG. 7. Transition probabilities as a function of n : $\theta = 0$ (blue), $\theta = \pi/4$ (red), and $\theta = \pi/2$ (green).

$\theta \neq 0$, convergence is reached as $n \rightarrow \infty$. In the absence of initial excited quanta, it is well known that longitudinal coupling ($\theta = 0$) does not contribute to the LZ transition. By gradually increasing the quanta number n , depending on the mixing angle, a more or less pronounced change in the final transition probability can be observed. Especially for a mixing angle of $\theta = \pi/4$, the effect is largest. Also, in this case, the energy exchange between the system and the oscillator is largest for large quantum numbers.

Finally, we investigate the transition for different oscillator frequencies for $n = 50$: slow oscillator $\omega = 0.2\omega_0$, intermediate oscillator $\omega = \omega_0$, and fast oscillator $\omega = 2\omega_0$, where $\omega_0 = \frac{\Delta}{4}$. Further parameters for the numerics are $N = 25$ and $M = 30$. The mixing angle is $\theta = \pi/4$. As shown in Fig. 8, the qubits start with the same initial probabilities and end with large transition probability in the case of a slow oscillator. As expected, the transition time is longer when the oscillator is slow and allows more transition to occur at intermediate times.

FIG. 8. Transition probabilities $P(t)$ as a function of ω : $\omega = 1 \times \omega_0$ (blue), $\omega = 0.2 \times \omega_0$ (green), and $\omega = 2 \times \omega_0$ (red), where $\omega_0 = \Delta/4$; mixing angle $\theta = \pi/4$.

V. CONCLUSIONS AND OUTLOOK

We have numerically investigated transition probabilities from the plus to the minus spin state, starting from eigenstates of the LZSM problem in the presence of an excited bosonic mode for $t \rightarrow -\infty$. The numerical workhorse was the multi-Davydov D_2 -Ansatz, and multiplicities up to 30 have been used to obtain converged results. A favorable expansion of the bosonic number state $|n\rangle$ in terms of coherent states along a suitably chosen circle has been employed. Although the circle's radius β is in principle arbitrary, numerical calculations show that correct results are obtained with reasonable numerical effort only if the radius is chosen as $\beta = \sqrt{n}$, in coincidence with Ref. 63.

The coupling to the harmonic oscillator contains diagonal ($\theta = 0$) as well as off-diagonal terms ($\theta = \pi/2$). With the avoided crossing (of the bare system) at $t = 0$, we found from a thorough convergence study that, especially for $\theta \neq 0$, in the numerics, we have to start from rather early times $t_0 \ll 0$. Furthermore, in order to compare results for different initial excitation number n of the bosonic mode, we had to scale the coupling strength with $1/\sqrt{n}$.⁴³ Then, we found convergence of the transition probability $P(t \rightarrow \infty)$ for large n . The asymptotic values are nontrivially dependent on the mixing angle θ . For $\theta = 0$, the diagonal coupling shows little effect on the transition probabilities at long times even in the presence of the initial excited quanta. For $\theta = \pi/4$, both channels of coupling are open, and it turns out that for large n , larger amounts of energy are exchanged between the spin and the oscillator as if one of the channels was closed. Furthermore, we have shown that also the oscillator frequency allows for a tuning of the final probability. If the oscillator is slower, more transitions occur at intermediate times, leading to larger transition probability at long times.

Furthermore, comparing to a straightforward quantum solution by basis set expansion for $\theta = \pi/2$, we found that even though large multiplicities are needed in the Davydov case, the Davydov numerics is still faster.

It would be an interesting topic for future studies to investigate if interference between the diagonal and off-diagonal coupling channels is responsible for the enhanced energy exchange between the spin and oscillator. This could be done by adding additional bath degrees of freedom with continuous spectral densities, leading to decoherence. Finally, on a more technical note, the finding that the sampling along the circle and the summation over multiplicity can be combined favorably could be extended toward studies of temperature dependent initial condition sampling.

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APPENDIX: PROPERTIES OF THE DISPLACEMENT OPERATOR AND THE LAGUERRE POLYNOMIALS

In the following, we collect properties of the displacement operator and its action on number states that are frequently needed in the

main text. In SI units, the Hamiltonian for a one-dimensional harmonic oscillator of mass m and frequency ω (up to a constant) is given by

$$\hat{H}_{\text{HO}} = \hbar\omega\hat{a}^\dagger\hat{a}, \quad (\text{A1})$$

with the creation and annihilation operators⁷¹

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\omega}\hat{p}\right), \quad (\text{A2})$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\omega}\hat{p}\right), \quad (\text{A3})$$

fulfilling the commutation relation

$$[\hat{a}, \hat{a}^\dagger] = 1. \quad (\text{A4})$$

The corresponding quantum mechanical displacement operator reads⁷²

$$\hat{D}[f(t)] = \exp\left[f(t)\hat{a}^\dagger - f^*(t)\hat{a}\right], \quad (\text{A5})$$

$$= \exp\left[-\frac{|f(t)|^2}{2}\right] \exp\left[f(t)\hat{a}^\dagger\right] \exp\left[-f^*(t)\hat{a}\right], \quad (\text{A6})$$

where the complex number $f(t)$ is related to the expectation values of the position and momentum operators $q_t = \langle\hat{q}\rangle(t)$ and $p_t = \langle\hat{p}\rangle(t)$ via

$$f(t) = \sqrt{\frac{m\omega}{2\hbar}}\left(q_t + \frac{i}{m\omega}p_t\right). \quad (\text{A7})$$

Using (A5), it can be shown most easily that the displacement operator is unitary

$$\hat{D}^{-1}[f(t)] = \hat{D}^\dagger[f(t)] = \hat{D}[-f(t)]. \quad (\text{A8})$$

In addition, the operators in the exponential could be disentangled, leading to (A6), by using the simplified Zassenhaus formula⁷³

$$\exp[\hat{A} + \hat{B}] = \exp[\hat{A}] \exp[\hat{B}] \exp\left\{-\frac{1}{2}[\hat{A}, \hat{B}]\right\}, \quad (\text{A9})$$

valid in the case that the operators $\hat{A}, \hat{B}$ commute with their commutator.

Furthermore, the displacement operator has the properties

$$\hat{D}^\dagger[f(t)]\hat{a}\hat{D}[f(t)] = \hat{a} + f(t), \quad (\text{A10})$$

$$\hat{D}^\dagger[f(t)]\hat{a}^\dagger\hat{D}[f(t)] = \hat{a}^\dagger + f^*(t), \quad (\text{A11})$$

which are frequently needed in the main text. They can be proven by using the Hadamard lemma⁷¹

$$\exp[\hat{B}]\hat{A}\exp[-\hat{B}] = \hat{A} + [\hat{B}, \hat{A}] + \frac{1}{2!}[\hat{B}, [\hat{B}, \hat{A}]] + \dots \quad (\text{A12})$$

In the main text, we will also need the time derivative of the displacement operator. It is given by

$$\frac{\partial\hat{D}[f]}{\partial t} = -\frac{\dot{f}f^* + f\dot{f}^*}{2}\hat{D}[f] + \dot{f}\hat{a}^\dagger\hat{D}[f] - \hat{D}[f]\dot{f}^*\hat{a}, \quad (\text{A13})$$

which was derived from the disentangled form (A6).

If applied to an excited state $|n\rangle$ of the harmonic oscillator, the displacement operator creates a so-called displaced number state.⁶¹ The overlap of two different such states is given by

$$\langle n|\hat{D}^\dagger[f]\hat{D}[g]|n\rangle = e^{-\frac{1}{2}(|f|^2+|g|^2)+f^*g}L_n(|g-f|^2), \quad (\text{A14})$$

with the Laguerre polynomials, L_n , the first three of which are

$$L_n(x) = \begin{cases} 1, & n = 0, \\ 1 - x, & n = 1, \\ 1 - 2x + \frac{1}{2}x^2, & n = 2. \end{cases} \quad (\text{A15})$$

Furthermore, for the equations of motion, we need expressions of the kind⁷⁴

$$\langle m|e^{z\hat{a}^\dagger}e^{-z^*\hat{a}}|n\rangle = \begin{cases} (-z^*)^{n-m}\sqrt{\frac{m!}{n!}}L_m^{n-m}(|z|^2), & \text{for } m \leq n, \\ z^{m-n}\sqrt{\frac{n!}{m!}}L_n^{m-n}(|z|^2), & \text{for } n \leq m, \end{cases} \quad (\text{A16})$$

with the associated Laguerre polynomials

$$L_n^k(x) = \sum_{i=0}^n \frac{1}{i!} \binom{k+n}{n-i} (-x)^i \quad (\text{A17})$$

that fulfill the 3-point-rule $L_n^k(x) = L_n^{k+1}(x) - L_{n-1}^{k+1}(x)$ and of which the above Laguerre polynomials are the special case $k = 0$. Then,

$$\langle n|\hat{a}^\dagger\hat{D}^\dagger[f(t)]\hat{D}[g(t)]|n\rangle = -(g-f)^*e^{-\frac{1}{2}(|f|^2+|g|^2)+f^*g}L_{n-1}^1(|g-f|^2) \quad (\text{A18})$$

is found. We note that for the derivation of the equations of motion also, the relation

$$\frac{d^\alpha}{dx^\alpha}L_n^k(x) = (-1)^\alpha L_{n-\alpha}^{k+\alpha}(x) \quad (\text{A19})$$

for the derivative of (generalized) Laguerre polynomials is helpful.

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