Landau-Zener transitions in a two-level system interacting with a harmonic oscillator at finite temperature

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We analyze the dynamics and final populations in a Landau-Zener problem for a two level system (or qubit) when this system interacts with one harmonic oscillator mode that is initially set to a finite-temperature thermal equilibrium state. The harmonic oscillator could represent an external mode that is strongly coupled to the qubit, e.g. an ionic oscillation mode in a molecule, or it could represent a prototypical uncontrolled environment. We analyze the qubit’s occupation probabilities at the final time in a number of different regimes, varying the qubit and oscillator frequencies, their coupling strength and the temperature. In particular we find some surprising non-monotonic dependence on the coupling strength and temperature.

I. INTRODUCTION

Landau-Zener (LZ) transitions occur when two energy levels cross, or more accurately experience an avoided crossing, as some external parameter is varied in time [1–4]. The system can then either stay in the same energy level that it occupied before the crossing, or it can experience a jump to the other level. Such a universal phenomenon is ubiquitous and has applications in various areas of quantum physics. Among the new areas where the physics of LZ transitions can play an important role are adiabatic quantum computation (AQC) [5] and amplitude spectroscopy in nanoscale circuits [6–8], and it could also play a role in the inter-molecular energy transfer in biological light-harvesting systems. In AQC, the parameters of a physical system (which can be called a quantum computer or annealer) are varied slowly such that the system transforms from an easy-to-prepare ground state into a ground state that contains the answer to a physical problem (or even a computational problem of non-physical nature). In biological light-harvesting systems, energy transfer between different parts of a molecule could be governed by molecular changes that act as driving fields for electronic motion.

The LZ problem in a closed system was solved soon after it was formulated over eighty years ago [1–4]. Physical systems, however, invariably interact with a surrounding environment. There have been numerous studies on the LZ problem in the presence of an environment [8–23], and some methods have produced accurate results in their regimes of validity. However, there is no method that is valid for all parameter regimes. In particular, the different methods typically have underlying assumptions justifying the validity of their mathematical formulation based on physical arguments. For example, one could make the assumption of a very short correlation or memory time in the environment’s degrees of freedom and use a Markovian approach. This approach would, however, break down when the environment’s correlation time is not short compared to the LZ time, which could occur when dealing with low-frequency noise.

Here we take a somewhat different approach. We numerically solve a rather simple physical problem composed of a single two-level system (to which we also refer as the qubit) coupled to a single harmonic oscillator. We can therefore be confident that our numerical calculations provide an accurate description of the problem as formulated. After obtaining the numerical results for the relatively simple problem, we comment on the physical meaning of these results and how they could apply for a system where the single harmonic oscillator is replaced by an environment with a large number of degrees of freedom.

The remainder of this paper is organized as follows: In Sec. III we describe the basic setup and introduce the corresponding Hamiltonian. In Sec. III we describe our numerical calculations. In Sec. IV we present the results of these calculations and discuss the interpretation of the results. Section V contains some concluding remarks.

II. MODEL SYSTEM AND HAMILTONIAN

We consider the basic LZ problem where the system of interest contains only two quantum states. As such, it can be described using the Pauli matrices $\sigma_\alpha$ with $\alpha = x, y$ or $z$. We use the basis states defined by the relations $\sigma_z |\uparrow\rangle = |\uparrow\rangle$ and $\sigma_z |\downarrow\rangle = -|\downarrow\rangle$.

In an isolated system, the LZ Hamiltonian is given by

$$H = -\frac{vt}{2} \sigma_z - \frac{\Delta}{2} \sigma_x,$$

(1)

where the time variable $t$ goes from $-\infty$ to $+\infty$, $v$ is the sweep rate and $\Delta$ is the minimum energy gap between the ground and excited states, which occurs at $t = 0$. At large negative times the ground and excited states asymptotically coincide with the states $|\uparrow\rangle$ and $|\downarrow\rangle$, respectively. The roles of these states are reversed at large positive times. At $t = 0$, the instantaneous ground and excited states are equal superpositions of the states $|\uparrow\rangle$ and $|\downarrow\rangle$. The LZ formula, which for example gives the probability for a system prepared in its ground state at $t \to -\infty$ to end up in the excited state at $t \to \infty$, is given by $P_{LZ} = \exp\{-\pi \Delta^2/(2v)\}$. In particular, for a
slow sweep (i.e. \( v/\Delta^2 \ll 1 \)), \( P_{LZ} \rightarrow 0 \) and a system that is initially prepared in the ground state has a high probability to remain in the ground state.

The LZ problem can be modified, or generalized, in order to take into account the effect of an uncontrolled external environment. Early studies on this problem used somewhat ad-hoc quantum master equations in order to incorporate dissipative processes in the dynamics \( \mathcal{E} \). Subsequent studies generally started with a specific model of the environment and derived approximate equations of motion for the system under certain approximations (see e.g. Refs. 10, 15, 21, 22). Because of computational convenience and physical relevance, the environment is commonly modeled as a large set of of harmonic oscillators, even if the microscopic details of the environment are not known. This approach has been applied successfully to the study of the LZ problem in a number of regimes. It is not possible, however, to obtain analytic results for this problem, and approximations that are valid for specific regimes are commonly made in order to calculate the effect of the large number of harmonic oscillators on the LZ probability. The strong-coupling and low-temperature regimes are particularly challenging for these methods.

Here we take a different approach to studying the effect of the environment on the LZ problem. We consider an environment composed of a single harmonic oscillator. Clearly this simple model will not be able to capture all the effects that occur in a complex environment. However, the simplicity of the model allows us to have confidence in the results of standard numerical simulations. Rather than having to make assumptions concerning the behaviour of the system at the beginning of the calculation, the difficult task is then shifted to the step of interpreting the numerical results and identifying in these results patterns and tendencies that one can expect to apply for an environment that contains a large number of degrees of freedom. It is also worth mentioning here that there can be cases where the largest environmental effects are caused by a single mode in the environment, in which case the results of this simple model become particularly relevant. Furthermore, the model that we analyze here is a minimal model of an LZ problem that incorporates extra degrees of freedom in addition to the single qubit, which allows us to discuss physical processes rather clearly.

We would like to note here that a related system, namely an LZ problem of a qubit coupled to a harmonic oscillator and an environment, was recently considered in Ref. 24. In that work, however, there is no minimum-gap term in the qubit’s Hamiltonian, and the avoided crossings arise as a result of the coupling between the qubit and the oscillator, rendering the system qualitatively different from the one that we consider here.

The Hamiltonian of the LZ problem with a single-mode environment and linear coupling is given by:

\[
H = -\frac{v t}{2} \hat{\sigma}_z - \frac{\Delta}{2} \hat{\sigma}_x + \hbar \omega \hat{a}\hat{a}^\dagger + g \hat{\sigma}_z \otimes (\hat{a} + \hat{a}^\dagger),
\]

where \( \omega \) is the characteristic frequency of the harmonic oscillator, \( \hat{a} \) and \( \hat{a}^\dagger \) are, respectively, the oscillator’s annihilation and creation operators, and \( g \) is the qubit-oscillator coupling strength. The energy level diagram of this problem is illustrated in Fig. 1.

We are interested in particular in the case of slow, nearly adiabatic passage. This case corresponds to the desired condition for obtaining a high transfer probability in problems where energy or quantum-state population is transferred between two systems via an LZ process; it is also the relevant regime for maximizing the success probability in an adiabatic quantum computation.

III. NUMERICAL CALCULATIONS

We numerically solve the time-dependent Schrödinger equation using the Hamiltonian given in Eq. (2). In these calculations we set the sweep rate \( v \) to the value that gives \( P_{LZ} = 0.1 \) (i.e., starting from the ground state, the two-level system ends up in the ground state with 99% probability). In other words, we choose a sweep rate that is close to the adiabatic limit in the absence of the coupling to the oscillator. We take three different values for the oscillator frequency: \( \omega/\Delta = 0.2 \) (low-frequency oscillator), 1 (intermediate regime), and 5 (high-frequency oscillator). We vary the coupling strength from \( g/\Delta = 0 \) to \( g/\Delta = 2 \), and we vary the temperature \( T \) from \( k_B T/\Delta = 0 \) to \( k_B T/\Delta = 5 \), where \( k_B \) is the Boltzmann constant.

We would like to simulate a finite-temperature environment (Note that the zero-temperature case allows an exact solution [15]). In order to incorporate the finite temperature into the calculation, the simulations are started.
in thermal equilibrium at a large negative value for the time variable. In this limit, the qubit and resonator are effectively decoupled from each other, except for energy shifts that they induce on each other. Furthermore, the qubit’s energy splitting is very large in the limit \( t \to -\infty \).

As a result, the qubit starts initially in its ground state \(|\uparrow\rangle\). The harmonic oscillator starts in a mixed thermal state according to the Boltzmann probability distribution with an average number of quanta \( k_B T / (\hbar \omega) \) for high temperatures (Note that the Boltzmann probability distribution extends up to several times this value). This estimate provides a minimum number of basis states that need to be included in the simulations, and it also sets a limit to the highest temperatures that can be reached in simulations with a given size of the Hilbert space. In particular for the lowest frequency and highest temperature that we consider, we use a Hilbert space with up to 1000 basis states.

After setting the initial state according to the Boltzmann distribution, we evolve the density matrix of the combined system in time according to the Schrödinger (or Liouville-von Neumann) equation. Note that this evolution is unitary, which is the reason why we can say that, in contrast to most other methods, we are not making any approximations or assumptions concerning the internal dynamics of the environment. The evolution is stopped at a sufficiently large and positive value of the time, such that further evolution would not have any noticeable effect on the occupation probabilities of the different states. At this final time, we examine the probability distribution, from which we can easily calculate the probability that the qubit remains in its ground state.

IV. RESULTS

The probability for the qubit to end up in the excited state at the final time as a function of temperature and coupling strength is plotted in Figs. 2-4. As expected from known results \([15]\), the final excited-state occupation probability \( P \) remains equal to 0.1 whenever the temperature or the coupling strength is equal to zero. Otherwise, the coupling to the oscillator causes this probability to increase. A common, and somewhat surprising, trend for all values of \( \hbar \omega / \Delta \) is the non-monotonic dependence on the coupling strength \( g \). As the coupling strength is increased from zero to finite but small values, \( P \) increases. But when the coupling strength is increased further, \( P \) starts decreasing (for all values of temperature). From the trends that can be seen in the figures, one can expect that in the limit of large \( g / \Delta \) (and assuming not-very-large values of \( k_B T / \Delta \)) the excited-state occupation probability will go back to its value in the uncoupled case, i.e. \( P = 0.1 \). This phenomenon is probably a manifestation of the superradiance-like behaviour in a strongly coupled qubit-oscillator system \([25]\). In the superradiant regime (i.e. the strong-coupling regime), the ground state is highly entangled exactly at the symmetry point (which corresponds to the bias conditions at \( t = 0 \) in the LZ problem), but very small perturbations will lead to an effective decoupling between the qubit and resonator with the exception of some state-dependent energy shifts. Indeed the maximum values of \( P \) reached in Figs. 3 and 4 occur at coupling strength values that are comparable to the expression for the superradiance tran-
sition point, namely $\sqrt{\hbar \omega / \Delta}$ (and in particular the peak in $P$ occurs around $\sqrt{\hbar \omega / \Delta}$). This relation does not apply in the case $\hbar \omega / \Delta = 0.2$, shown in Fig. 2. In this case, the peak occurs when the coupling strength $g$ is comparable to the minimum gap $\Delta$. It is in fact quite surprising that the excitation peak in the case $\hbar \omega / \Delta = 0.2$ occurs at a higher coupling strength than that obtained in the case $\hbar \omega / \Delta = 1$. In order to investigate this point further, we tried values close to $\hbar \omega / \Delta = 1$ and found that this value gives a minimum in the peak location (i.e. the peak in $P$ when plotted as a function of $g/\Delta$).

Another feature worth noting is the dependence of $P$ on temperature close to zero temperature. As can be seen clearly in Figs. 3 and 4 the initial increase in $P$ probably follows an exponential function that corresponds to the probability of populating the excited states in the harmonic oscillator (and the same dependence is probably present but difficult to see because of the scale of the $x$ axis in Fig. 2). After this initial slow rise, and in particular when $k_B T \gtrsim \hbar \omega$, we see a steady rise that in the case of Fig. 2 can be approximated as a linear increase in $P$ when $k_B T > \hbar \omega$. Importantly, the slope of this increase can be quite large for intermediate $g$ values. As can be seen in Fig. 4 even when the temperature is substantially smaller than the qubit’s minimum gap $\Delta$, the initial excitation of the low-frequency oscillator (stemming from the finite temperature) can cause a large increase in the qubit’s final excited-state probability. This result is in contrast with the exact result of Ref. [15] stating that at zero temperature the qubit’s final excited-state probabil-
ity is given by $P_{LZ}$ regardless of the value of $g$. The typical temperature scale at which deviations from the LZ formula occur can therefore be much lower than $\Delta/k_B$. This result is relevant for adiabatic quantum computing, where one might think that having a minimum gap that is large compared to the temperature will provide automatic protection for the ground state population against thermal excitation. The excitations in the oscillator at the initial time are in some sense up-converted into excitations of the qubit as a result of the sweep through the avoided crossing.

We can also see in Fig. 2 that for $g/\Delta \gtrsim 1$ the temperature dependence is non-monotonic. In particular, for low temperatures we obtain the intuitively expected increase in excitation probability with increasing temperature, but this trend reverses for higher temperatures. In order to investigate this feature further, we calculate the qubit’s final excited-state probability as a function of the number $n$ of excitation quanta present in the initial state of the oscillator (Note that this calculation differs from earlier ones in that here we do not use the Boltzmann distribution for the oscillator’s initial state). The results are plotted in Fig. 5. These results explain the non-monotonic dependence on temperature. For intermediate values of $g/\Delta$, there is a peak at a small but finite excitation number followed by a steady decrease. As the temperature is increased from zero, the qubit’s final excited-state probability samples the probabilities for increasingly higher excitation numbers, and a peak at intermediate values of temperature is obtained. Note that for large excitation numbers, the increase in $P$ as a function of $n$ resumes, and this increase will also be reflected in the temperature dependence.

We note that recent theoretical studies \cite{21, 22} have reported non-monotonic dependence of the excitation probability as a function of sweep rate $v$. However, that dependence was generally oscillatory, and we suspect that it has a different origin from the behaviour obtained in the present study. We expect that similar oscillatory behaviour would be obtained if we varied $v$ in our calculations. As mentioned in Sec. II, however, here we are mainly interested in the almost-adiabatic regime, and we have therefore not analyzed the $v$-dependence in our calculations.

In addition to solving the Schrödinger equation, we have performed calculations where we assume that there is no quantum coherence between the different LZ pro-
cesses (Note here that in the coupled qubit-oscillator system the single relevant avoided crossing is replaced by a complex network of crossings). Under this approximation, we only need to calculate the occupation probabilities of the different states, and these probabilities change (according to the LZ formula) only at the points of avoided crossing. This approach greatly simplifies the numerical calculations because the locations and gaps for the different avoided crossings can be determined easily (see Fig. 1). The results are shown in Fig. 5. The results of this calculation agree generally well with those obtained by solving the Schrödinger equation when \( \hbar \omega / \Delta = 1 \). For \( \hbar \omega / \Delta = 5 \), the transition-probability-based calculation consistently underestimates the excited-state probability, but the overall dependence on temperature and coupling strength is remarkably similar to that shown in Fig. 5. The most striking deviation from the results obtained by solving the Schrödinger equation are seen in the case \( \hbar \omega / \Delta = 0.2 \) (i.e. the case of a low-frequency oscillator). In the transition-probability-based calculation, there is a rather high peak at small values of the coupling strength (and sufficiently high temperatures), and the excited-state probability starts decreasing when the coupling strength \( g \) becomes larger than \( \hbar \omega \). In the fully quantum calculation, however, the peak is located at a much higher value, somewhere between 0.5 and 1 depending on the temperature.

The fact that the transition-probability-based calculation generally gives results different from those given by the fully quantum calculation is an indication that quantum coherence and interference between multiple LZ processes plays a role in determining the excited state probability. In this context we note that the avoided crossings occur at instances separated by time intervals \( \tau_{\text{separation}} = h \omega / v \) (with an infinite number of avoided crossings occurring simultaneously at each one of these instances), and the time duration over which an LZ mixing process occurs (in the almost-adiabatic regime) is given by \( \tau_{\text{LZ}} \sim \Delta / v \) \( \tau_{\text{LZ}} \sim \hbar \omega / \Delta \) (Note that most of the avoided crossing gaps are much smaller than \( \Delta \), and this estimate is therefore a conservative one). The ratio between these two time scales is then given by \( \tau_{\text{separation}} / \tau_{\text{LZ}} \sim \hbar \omega / \Delta \). In other words, when \( \hbar \omega / \Delta \) is small the different LZ processes will overlap in time, and it is not too surprising that the transition-probability-based calculation gives incorrect predictions in this case. It is somewhat surprising, however, that when \( \hbar \omega / \Delta = 1 \) the two calculations agree quite well and then in the regime \( \hbar \omega / \Delta > 1 \) (in particular at \( \hbar \omega / \Delta = 5 \)) the effect of quantum interference between the LZ processes can again be seen in the final excited-state probability.

We now consider how the above results translate to results that apply to a large environment containing a large number of degrees of freedom. When there is no single dominant mode in the environment, the coupling between the qubit and each individual mode is typically weak. The difference between this situation and the single-mode model is clearly demonstrated by considering the strong-coupling regime. While (as our results show) strong coupling to a single mode results in a reduced effect of that mode on the qubit, it is most likely that this is no longer the case when the qubit is coupled strongly to an uncontrolled environment containing a large number of independent modes with the coupling to each individual mode in the environment being weak. The weakening of the environmental effects with increased coupling strength in the case of a single mode is most likely related to the energy level structure and the possible paths that the system can follow in a sequence of LZ processes. The energy level structure and the possible LZ transitions are vastly different when the strong coupling to the environment is caused by the large number of modes in the environment. It would be more plausible that in this case one should focus on the small \( g / \Delta \) region of the results discussed above, take the contributions of the individual environment modes and add up these small contributions. In this case an increase in coupling strength would result in an increase in the excited state probability, as would be intuitively expected. We therefore emphasize that the result of non-monotonic behaviour with increasing coupling strength should be thought of as a result pertaining to the case with a single dominant mode in the environment. Another area where we can try to extract from our results statements concerning a large environment occurs in the regime of low temperatures in the context of AQC. It is known the the minimum gap in AQC decreases with increasing system size. This scaling property is typically discussed in relation to the time needed to ensure adiabatic evolution of the quantum annealer. It turns out that coupling to an environment at zero temperature does not affect the excitation probability in an AQC algorithm, since at zero temperature the LZ probability remains equal to its value for an isolated system (a result that is itself quite counter-intuitive) \[15\]. The fact that at finite temperatures the excitation probability increases and that low-frequency modes in particular can substantially modify the excitation probability even at temperatures much lower than the minimum gap means that the coupling to the environment also needs to be considered more carefully in future studies on AQC.

V. CONCLUSION

We have investigated the problem of a two-level system undergoing an LZ passage through an avoided crossing while being coupled to a finite-temperature harmonic oscillator. We have found a number of counter-intuitive results, including non-monotonic dependence of the final excitation probability as a function of temperature or qubit-oscillator coupling strength. We have provided physical explanations for these phenomena. The physical mechanisms at play include modifications to the avoided crossing structure related to the formation of highly correlated energy eigenstates as well as quantum coherence.
between multiple LZ processes.

We emphasize that our results are of interest even in the single-oscillator case, both because they pertain to a model system that allows a clear discussion of the physical mechanisms involved and because certain systems in nature are accurately described by the model of a single qubit coupled to a single oscillator. From the open-system point of view, our results can be seen as a study on a prototypical environment. In this spirit, we have discussed how our results can be used to make statements concerning the LZ problem in the presence of a large environment and the implications of these results to topics of current interest, such as adiabatic quantum computing.

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