Influence of Dissipation on the Landau-Zener Transition

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The quantum dynamics of the Landau-Zener transition in a dissipative environment is studied and analytical results for the transition probability are given in terms of temperature, coupling strength, and the Landau-Zener time. For short Landau-Zener time there is no effect of dissipation. In the opposite limit we distinguish various temperature regimes: The adiabatic limit is shown to be restricted to low temperatures and no effect of dissipation is present at zero temperature. At intermediate temperatures thermal transitions dominate for weak coupling and high temperatures correspond to the strong coupling limit.

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We consider the explicitly time-dependent situation in which the energy levels of a quantum-mechanical system are brought close together in the course of time by external means, so that transitions between the levels take place and enable us to study the effect of a dissipative environment on the transition probability. This level crossing problem appears in numerous contexts not only in physics, but also in chemistry, through its relevance to chemical reaction kinetics,[1] as well as in biophysics.[2] In physics the problem is encountered widely from the solar neutrino puzzle[3] to numerous situations in atomic and solid-state physics: Nuclear magnetic resonance,[4] aspects of the behavior of laser irradiated atoms,[5] atomic collisions,[6] atoms scattering off surfaces,[7] and dielectric breakdown[8] are all well-known examples. However, the question has also gained renewed interest in view of its relevance to mesoscopic systems, for example, the effect of dissipation of Zener tunneling and the resulting influence on the dynamics of an electron in a mesoscopic ring.[9] The question of the effect of dissipation on the quantum dynamics of a macroscopic variable has recently received much interest in the context of macroscopic quantum tunneling and coherence,[10] and in this respect the present paper addresses questions relevant for the possible observability of Bloch oscillations in Josephson junctions, insofar as this effect can be considered the counterpart of an electron moving in a crystal under the influence of an external electric field.

In the absence of coupling to the environment the nonadiabatic transition we consider is customarily referred to as the Landau-Zener transition. Quantitatively this level crossing is described by the two-dimensional spin problem as given, in terms of the Pauli matrices, by the time-dependent system Hamiltonian $H_s(t) = vt\sigma_z + \Delta\sigma_x$. For the description of the environment we take harmonic oscillators as represented by the bath Hamiltonian $H_B = \sum_\alpha \hbar\omega_\alpha (a_\alpha^\dagger a_\alpha + \frac{1}{2})$ and for the interaction between system and environment we take the coupling linear[11] in the bath coordinate X, $H_I = \sigma_z X$, $X = \sum_\alpha \lambda_\alpha (a_\alpha^\dagger + a_\alpha)$. Here $a_\alpha^\dagger$ and a_α denote the boson creation and annihilation operators corresponding to the frequency ω_α and λ_α is the coupling constant.[12] Our total Hamiltonian is thus the spin-boson Hamiltonian with a time-dependent bias

$$H(t) = H_s(t) + H_B + H_I . \tag{1}$$

The model is specified by the energy gap 2Δ between the two levels and the effective coupling to the environment as described by the spectral function $J(\omega) = (2/\hbar)^2 \sum_\alpha \lambda_\alpha^2 \delta(\omega - \omega_\alpha)$ and as external parameters we have the sweeping rate v, describing the effect of the external force, and the temperature T.

We now pose the problem to be solved: At a remote time t_0 (which for all purposes can be taken to be $t_0 = -\infty$) we assume that our initial state is described by the initial statistical operator[13] $\rho_1 = |\uparrow\rangle\langle\uparrow|\rho_B$, where ρ_B is the equilibrium statistical operator for the bath described by $\exp(-H_B/k_B T)$. The system, that is the spin, is then initially in the ground state and we then ask for the probability P that the system in the far future is in its excited state while the bath is assumed unobserved. For the transition probability P we then have the expression

$$P = \mathrm{Tr}[\rho_B P_T U^+(\infty, -\infty) P_T U(\infty, -\infty)] , \tag{2}$$

where $U(t,t') = T\exp[(-i/\hbar)\int_{t'}^{t} d\bar{t}\, H(\bar{t})]$ is the evolution operator (T denoting time ordering) corresponding to the total Hamiltonian $H(t)$, P_T projects onto the spin-up state, and $+$ denotes Hermitian conjugation. Certain aspects of the problem have previously been studied from a phenomenological point of view.[5,7] We shall perform a microscopic calculation and employ the real-time quantum-dynamical technique[14] as this general method allows calculations for externally driven systems at finite temperatures.

We start by calculating the transition probability in the limit where the system's degrees of freedom traverses the transition region slowly, that is, the Landau-Zener time $\tau_{LZ} = \Delta/v$ is much smaller than $\hbar/\Delta$ or in terms of the dimensionless parameter $\gamma = \Delta^2/2\hbar v$, $\gamma \gg 1$. The calculation is facilitated by rotating around the y axis in spin space through the angle $\chi(t) = -\operatorname{arccot}(vt/\Delta)$ to obtain the Hamiltonian $\mathcal{H}(t)$ in the adiabatic frame

$$\mathcal{H}(t) = H_0(t) + H_1(t)\,, \tag{3}$$

where $H_0(t) = -\epsilon_t\sigma_z + f(t)\sigma_z X + H_B$ is diagonal in spin space, and $H_1(t) = (\hbar v\Delta/2\epsilon_t^2)\sigma_y + (\Delta/\epsilon_t)\sigma_x X$. We have introduced the adiabatic energy $\epsilon_t = [(vt)^2+\Delta^2]^{1/2}$ and the abbreviated notation $f(t) = vt/\epsilon_t$. The first term in $H_1(t)$ describes the correction to adiabaticity as reflected by the unitary transformation to the adiabatic frame, $R(t) = \exp[\frac{1}{2}i\chi(t)\sigma_y/\hbar]$, being time dependent. The environment coupling to σ_z is now time dependent and weaker in the transition region as compared to the original frame, but in this region we now get an additional coupling to σ_x, represented by the second term in $H_1(t)$, which causes flips between the up and down spin states accompanied by phonon emission and absorption. In the adiabatic limit we only need to consider one flip and upon getting rid of the explicit appearance of the spin operators by utilizing the fact that $H_0(t)$ is diagonal in spin space we get the following expression for P:

$$P = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \exp\left[-(2i/\hbar)\int_{t_2}^{t_1} dt\,\epsilon_t\right]\langle U_1(t_1,t_0)B[\epsilon_{t_1},X(t_1)]U_{-1}(t_1,t_2)B^+[\epsilon_{t_2},X(t_2)]U_1(t_2,t_0)\rangle\,, \tag{4}$$

where we use the shorthand notations $B[\epsilon_t,X(t)] = \Delta v/2\epsilon_t^2 + i(\Delta/\hbar\epsilon_t)X(t)$ and $U_{\pm 1}(t,t') = T\exp[(\pm 1)(-i/\hbar) \times \int_{t'}^{t} d\bar{t}\, f(\bar{t})X(\bar{t})]$, where $X(t) = \exp(iH_B t/\hbar)X\exp(-iH_B t/\hbar)$ has been introduced, and the bracket $\langle\cdots\rangle$ is short for $\mathrm{tr}(\rho_B\cdots)$, where tr denotes the trace over the environmental degrees of freedom only.

We now employ the real-time dynamical technique by introducing the generating functional for the environmental coordinate X along the closed time path c, extending from $-\infty$ to $+\infty$ and back to $-\infty$ along the real axis[14,15] $Z[\zeta] = \langle T_c \exp[(-i/\hbar)\int_c d\tau\,\zeta(\tau)X(\tau)]\rangle$. Here τ resides on c and T_c denotes the contour ordering operator.

Employing functional differentiation we can then express Eq. (4) as

$$P = 2\,\mathrm{Re}\int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2 \exp\left[-(2i/\hbar)\int_{t_2}^{t_1} dt\,\epsilon_t\right] B\{\epsilon_{t_2}, i\hbar[\delta/\delta\zeta_1(t_2)]\}B^+\{\epsilon_{t_1}, i\hbar[\delta/\delta\zeta_1(t_1)]\}Z[\zeta]\,|_{\zeta=\zeta^0}\,,$$

provided that after the functional differentiation we insert the proper "force" $\zeta = \zeta^0$. On the forward part (indicated by subscript 1 on ζ) of the contour we shall choose $\zeta_1^0(t) = f(t)[1 - 2\{\Theta(t-t_1) - \Theta(t-t_2)\}]$, where Θ denotes the step function and on the return part (indicated by subscript 2 on ζ) we shall choose $\zeta_2^0(t) = f(t)$. The generating functional Z is according to Wick's theorem given by

$$Z[\zeta] = \exp\left[(i/2\hbar^2)\int_c d\tau \int_c d\tau'\,\zeta(\tau)D(\tau,\tau')\zeta(\tau')\right],$$

where we have introduced the contour ordered Green's function, $D(\tau,\tau') = -i\langle T_c[X(\tau)X(\tau')]\rangle$.[16]

We can now evaluate the integrand of Eq. (4) and obtain

$$P = \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2\, A(t_1,t_2)\exp[i\Phi(t_1,t_2)]\,. \tag{5}$$

Here $\Phi(t_1,t_2) = \phi_0(t_1) - \phi_0(t_2) + \phi(t_1,t_2)$, $A(t,t') = (v\Delta/2\epsilon_t\epsilon_{t'})^2 B(t,t')$, where

$$B(t,t') = (2\epsilon_t\epsilon_{t'}/v\Delta)^2[a(t',t)a(t,t') + (i/\hbar^2)D_{11}(t,t')]Z(t,t')$$

is given in terms of the following:

$$a(t,t') = (v\Delta/2\epsilon_t^2) + i(\Delta/\hbar^2\epsilon_t)\int_{-\infty}^{\infty} d\bar{t}\, f(\bar{t})D^R(t,\bar{t})\,,$$

$$Z(t,t') = \exp\left[(-i/4)\int_{t'}^{t} d\bar{t}\int_{t'}^{t} d\bar{t}'\, f(\bar{t})D^K(\bar{t},\bar{t}')f(\bar{t}')\right],$$

$$\phi(t_1,t_2) = -2\int_{-\infty}^{t_1} dt \int_{-\infty}^{t_2} dt' \int_0^{\infty} d\omega\, J(\omega) f(t) \times \sin[\omega(t-t')]f(t')\,,$$

and $\phi_0(t) = -(1/\hbar)\int_{-\infty}^{t} dt'\,\epsilon_{t'}$. The Green's functions appearing are the retarded, Keldysh, and the usual time ordered.[16]

In the absence of coupling to the environment the integrals over t_1 and t_2 are uncoupled and dominated, provided that the "adiabatic" parameter γ satisfies $\gamma \gg 1$, by the stationary phase point of ϕ_0 which for the integral over t_1 (t_2) is $i\tau_{\mathrm{LZ}}$ $(-i\tau_{\mathrm{LZ}})$. If $\eta \ll \hbar\omega_c/\Delta$ then this is also the case in the presence of the environment.[17] Evaluating the transition probability in the stationary-phase approximation gives $P = B(i\tau_{\mathrm{LZ}}, -i\tau_{\mathrm{LZ}})\exp[i \times \phi(i\tau_{\mathrm{LZ}}, i\tau_{\mathrm{LZ}})]P_0$, where $P_0 = (\pi/4)^2\exp(-2\pi\gamma)$ is the bare transition probability within the same approximation. Evaluating B and ϕ at the stationary point we obtain the adiabatic result

$$P = P_0 \exp[\mathcal{E}(T,\tau_{\mathrm{LZ}})]\,, \tag{6}$$

where

$$\mathcal{E}(T,\tau_{\mathrm{LZ}}) = 2\pi(\tau_{\mathrm{LZ}})^2 \int_0^{\infty} d\omega\, J(\omega)n(\omega)I_1^2(\omega\tau_{\mathrm{LZ}})\,.$$

Here n is the Bose function and I_1 is the modified Bessel function. For the adiabatic result to be valid we must require not only the adiabatic criterion in the absence of the environment be satisfied, $\gamma \gg 1$, but also that the temperature T is smaller than $\Delta/4\gamma k_B$. Otherwise the term involving D^K will be ultraviolet divergent and the assumption of Z being a smoothly varying function, necessary for the stationary-phase method to be applicable, ceases to be valid. Surprisingly, we find that in the adiabatic limit at zero temperature the tunneling probability is not affected by the presence of the coupling to the environment as $\mathcal{E}(T=0,\tau_{LZ})$ is equal to zero for any physical choice of the spectral function.[18] The temperature dependence originally appears in B in the form $\coth(\hbar\omega/2k_BT)=2n(\omega)+1$. The latter quantum noise term is cancelled by the term $\exp[i\phi(i\tau_{LZ},-i\tau_{LZ})]$ describing the systematic force provided by the bath. The quantum noise term alone leads to an increase in the tunneling probability; this is due to the circumstance that the exponentially small bare tunneling probability is a result of delicate destructive interference between amplitudes which in the presence of the quantum noise is partially upset. The cancelling systematic force term effectively renormalizes the adiabatic parameter γ, and constitutes a combined renormalization of the energy gap and the sweeping rate.[19]

In the calculation of the transition probability in the slow-passage limit we did not explicitly have any weak coupling restrains and for instance found a divergent result beyond the temperature $k_BT=\Delta/4\gamma$ independent of the coupling strength. Now we treat the effect of the environment on the system perturbatively and by working explicitly in the coupling strength we achieve the possibility of exploring the weak coupling, but higher-temperature regime. The zeroth-order problem given by $H_s(t)+H_B$ is exactly solvable in terms of the parabolic cylinder functions[6,20] and treating H_I as a perturbation we can calculate the transition probability P from Eq. (2), $P=\exp(-2\pi\gamma)+\Delta P$. For the lowest-order correction in the coupling ΔP we can, in the slow-passage limit, $\gamma\gg 1$, and at temperatures $k_BT>\Delta/\ln\gamma$, extract the leading order $[O(1/\ln\gamma)]$ behavior by using the asymptotic expansions of the parabolic cylinder functions[21] and obtain for the lowest-order correction to the transition probability,

$$\Delta P=4\pi\gamma^{3/2}(\hbar/\Delta)J(2\Delta/\hbar)n(2\Delta/\hbar). \tag{7}$$

Thus, we easily obtain a prediction for the region where the environment-dependent contribution ΔP dominates the bare tunneling probability.

With the above results we have the following picture of the slow-passage, weak coupling limit: At low temperatures, $k_BT\ll\Delta/4\gamma$, the transition takes place via quantum tunneling, and the precursor effect on P of dissipation is of the form $P=P_0[1+(12\pi/\hbar)\eta(\gamma k_BT/\Delta)^4]$.[17] At temperatures $\Delta/\gamma<k_BT<\Delta$ thermally assisted transitions across the energy gap take place, which for these intermediate temperatures has the form of thermal activation across the energy gap whereas at higher temperatures, $k_BT>\Delta$, the transition probability is linear in temperature. At high enough temperatures, $k_BT\gg\Delta/\eta\gamma$, the perturbative result is invalid reflecting that this limit effectively is the strong coupling limit where the transition probability, as shown later, saturates to the value $\frac{1}{2}$.

The fast-passage limit, $\gamma\ll 1$, turns out to be simple in that to lowest order in γ there is no influence of the bath[22] irrespective of the coupling strength so that the transition probability is given by

$$P=1-2\pi\gamma. \tag{8}$$

To investigate the strong coupling limit we start from the exact expression for the transition probability P that emerges from Eq. (2) when one first calculates the matrix elements with respect to the spin degrees of freedom and subsequently performs the trace over the bath degrees of freedom.[23] In general this expression is too complicated to allow further progress, however, in the strong coupling limit we can apply the so-called noninteracting blip approximation.[24] For the transition probability we then obtain[25]

$$P=1+\tfrac{1}{2}\sum_{n=1}^{\infty}(-1)^n\int_{-\infty}^{\infty}dt_{2n}\int_{-\infty}^{t_{2n}}dt_{2n-1}\cdots\int_{-\infty}^{t_2}dt_1[g(t_2,t_1)+h(t_2,t_1)]\prod_{j=2}^{n}g(t_{2j},t_{2j-1}), \tag{9}$$

where the functions g and h are given by

$$g(t_2,t_1)=(2\Delta/\hbar)^2\cos[(v/\hbar)(t_2^2-t_1^2)]\cos[Q_1(t_2-t_1)]\exp[-Q_2(t_2-t_1)],$$

$$h(t_2,t_1)=(2\Delta/\hbar)^2\sin[(v/\hbar)(t_2^2-t_1^2)]\sin[Q_1(t_2-t_1)]\exp[-Q_2(t_2-t_1)].$$

In the strong coupling limit, $\eta(\omega_c)^{1-s}\gg 1$, the exponential suppression of g and h by the factor containing $Q_2(t)$ limits the range of integration to small time differences resulting in the simplification that we [in Eq. (9)] can neglect the term containing h. Similarly, after a change of variables[26]

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

we note that we can drop the quadratic terms in the y_k's in the expression

$$t_{2j}^2-t_{2j-1}^2=2y_k\left[x_k-\tfrac{1}{2}y_k+\sum_{m=1}^{k}y_m\right]$$

and have for the transition probability

$$P=1+2(\Delta/\hbar)^2\sum_{n=1}^{\infty}(-1)^n\int_{-\infty}^{\infty}dx_1\int_{x_1}^{\infty}dx_2\cdots\int_{x_{n-1}}^{\infty}dx_n\int_0^{\infty}dy_1\cdots\int_0^{\infty}dy_n\prod_{k=1}^{n}\cos[(2v/\hbar)y_kx_k]$$
$$\times\cos[Q_1(y_k)]\exp[-Q_2(y_k)].$$

The integral can now be performed and we obtain

$$P=\tfrac{1}{2}[1+\exp(-4\pi\gamma)]\,. \qquad (10)$$

This result is valid for all temperatures and all values of the "adiabatic" parameter γ in the strong coupling regime. The result, Eq. (10), has also been obtained by the phenomenological approach of Ref. 5, where it appears as the high-temperature limiting case. Our derivation, furthermore, shows that high temperatures correspond to strong coupling, thereby confirming the phenomenological approach in this limit.

In conclusion, we have performed a first-principle study of the effect of dissipation on the level crossing transition within the Landau-Zener model. In addition to establishing the adiabaticity criterion, analytical results have been obtained for the limiting cases. In the fast-passage limit the transition probability is not influenced by the presence of the bath for all temperatures and all values of the coupling strength η. In the strong coupling limit we have obtained the transition probability for all temperatures and all γ. In the weak coupling and slow-passage limit we obtain the following: at zero temperature no effect of the environment, only unmodified quantum tunneling. At low temperatures $k_BT \ll \Delta/\gamma$, the exponent increases with temperature as a power and at higher temperatures, the transition probability depends on the number of bosons present at the energy gap. At high temperatures the transition probability approaches the strong coupling value $\frac{1}{2}$.

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[18]Y. Gefen, E. Ben-Jacob, and A. O. Caldeira [Phys. Rev. B **36**, 2770 (1987)] reach the opposite conclusion. The difference is due to the use of their Eq. (2.28) for the adiabatic energy difference in the phase factor which is insufficient as it neglects the equally important coupling contribution to the adiabatic energy.

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[23]The expression that emerges is of the form in Eqs. (4)–(7) of S. Chakravarty and A. J. Leggett [Phys. Rev. Lett. **52**, 5 (1984)] except for a straightforward generalization to our case of a time-dependent bias.

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