The Landau-Zener Model with Decoherence:
The case $S=1/2$

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Abstract. We study the dynamics of a spin coupled to an oscillating magnetic field, in the presence of decoherence and dissipation. In this context we solve the master equation for the Landau-Zener problem, both in the unitary and in the irreversible case. We show that a single spin can be “magnetized” in the direction parallel to the oscillating bias. When decay from upper to lower level is taken into account, hysteretic behavior is obtained.

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1. Introduction

This paper concerns the dynamics of a driven two-level system with decoherence and dissipation. Such a simple quantum-mechanical problem has been studied in various contexts, as, e.g., nuclear and atomic physics. What follows is predominantly motivated by molecular magnets and quantum information, as long as these topics suggest new perspectives to the old problem.

The perspective of a comprehensive theory of molecular magnets stimulated a large amount of work. Rather than giving an extensive review, we merely quote a few topics in this area. A 1/2 spin (the central spin) has been introduced in modeling the macroscopic spin tunneling (for a short review see, e.g., Ref.[1]); dissipative spin reversal, incoherent Zener tunneling, decoherence were also considered [2, 3, 4].

Work more directly related to ours can be found in Refs. [7, 8, 6]. In classifying the behaviors of our system, we find effects such as single spin dynamical magnetization and hysteresis; the meaning of these terms will be made clear in the sequel.

In the presence of an oscillating external field, the evolution is characterized by a sequence of level-crossings, where the Landau-Zener (L-Z) model [9, 10] applies, separated by intervals of “normal” evolution.

We classify the dynamics from the behavior in the L-Z regime and in the “normal” regime. In order to do that, we first solve the Landau-Zener problem in the master equation for the density matrix. This is done both in the unitary and in the irreversible case.

Our starting point is Kraus’s [13] representation theorem, for the density matrix of a two-level system: a short reminder of the theory is given in Sections 2,3; for the sake of completeness, in Appendix I we recall the conditions for the complete positivity of the evolution [12].

In Section 4 we discuss the unitary case by means of qualitative methods. We examine high frequency fields as well as quasistatic fields. We show that a “magnetized” spin can be sustained, in the direction of a zero-average oscillating bias.

The non-unitary case, where dissipation and decoherence are taken into account, is discussed in Section 5. We show that the L-Z problem can be solved in the irreversible case; the solution is explicit for two-level systems.

We find the lowest order (in the 1/t expansion) renormalizations of the dissipation and decoherence parameters: the non-unitary processes do not modify the scattering properties of the solution at the level crossings. After analyzing the single-spin “magnetization” with decoherence, we take into account the relaxation from the upper to the lower level. In section 6 we show that an oscillating external field gives rise to hysteretic behavior.
2. Master equation for the two-level system

We start with the following master equation, for the density matrix of a two-level system:

\[ \dot{\rho} = -\frac{i}{\hbar}[H, \rho(t)] + \frac{1}{2} \sum_{i,j=1}^{3} A_{ij} ([\sigma_i, \rho(t) \sigma_j^+] + [\sigma_i \rho(t), \sigma_j^+]) \]  

(1)

where \( H \) is associated with reversible dynamics, the matrix \( A \) is Hermitean and the \( \sigma_i \)'s are the Pauli matrices.

The Hamiltonian is parametrized by 3 real parameters:

\[ H = \frac{1}{2} \{ \Delta \sigma_1 + \Delta' \sigma_2 + \omega_0 \sigma_3 \} \]  

(2)

and further 9 real parameters label the \( 3 \times 3 \) hermitean matrix \( A_{ij} \).

Notice that this is consistent with the Kraus representation \[13\], where the time evolution of a two-level system is characterized by 12 real parameters.

As it is well known, the coefficients of \( A \) are the correlation functions of the macrosystem coupled with the spin.

We then write Eq. 1 in the standard representation:

\[ \rho(t) = \frac{1}{2} \left[ \begin{array}{cc} 1 + Z & X - iY \\ X + iY & 1 - Z \end{array} \right] \quad \mathbf{v} = \left[ \begin{array}{c} X \\ Y \\ Z \end{array} \right] \]  

(3)

we have:

\[ \dot{\mathbf{v}}(t) = M \mathbf{v}(t) + \mathbf{C} \]  

(4)

The unitary contribution in \( M \) has the form:

\[ \begin{bmatrix} \dot{X} \\ \dot{Y} \\ \dot{Z} \end{bmatrix}_H = \begin{bmatrix} 0 & -\omega_0 & \Delta' \\ \omega_0 & 0 & -\Delta \\ -\Delta' & \Delta & 0 \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} \]  

(5)

and the decoherence and dissipation processes give:

\[ \begin{bmatrix} \dot{X} \\ \dot{Y} \\ \dot{Z} \end{bmatrix}_D = \begin{bmatrix} -2(A_{22} + A_{33}) & (A_{12} + A_{21}) & (A_{13} + A_{31}) \\ (A_{12} + A_{21}) & -2(A_{33} + A_{11}) & (A_{23} + A_{32}) \\ (A_{13} + A_{31}) & (A_{23} + A_{32}) & -2(A_{11} + A_{22}) \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} + \begin{bmatrix} 2i(A_{23} - A_{32}) \\ 2i(A_{31} - A_{13}) \\ 2i(A_{12} - A_{21}) \end{bmatrix} \]

or:

\[ \dot{\mathbf{v}}_D = D \mathbf{v} + \mathbf{C} \]

In Eq. 4, the explicit form of \( M \) is made more readable by letting:

\[ \gamma_1 = 2(A_{22} + A_{33}) \quad \gamma_2 = 2(A_{33} + A_{11}) \quad \gamma_3 = 2(A_{11} + A_{22}) \]
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\[ \alpha = (A_{12} + A_{21}) \quad \beta = (A_{13} + A_{31}) \quad \gamma = (A_{23} + A_{32}) \]
\[ C_1 = 2i(A_{23} - A_{32}) \quad C_2 = 2i(A_{31} - A_{13}) \quad C_3 = 2i(A_{12} - A_{21}) \]

so that:

\[ \begin{bmatrix} \dot{X} \\ \dot{Y} \\ \dot{Z} \end{bmatrix} = \begin{bmatrix} -\gamma_1 & \alpha - \omega_0 & \beta + \Delta' \\ \alpha + \omega_0 & -\gamma_2 & \gamma - \Delta \\ \beta - \Delta' & \gamma + \Delta & -\gamma_3 \end{bmatrix} \begin{bmatrix} X \\ Y \\ Z \end{bmatrix} + \begin{bmatrix} C_1 \\ C_2 \\ C_3 \end{bmatrix} \]

(6)

3. Geometrical interpretation of the 12 parameters

The phase space of the system is a Poincaré surface, undergoing elementary instantaneous transformations, according with $M$ and $C$.

More specifically, while the antisymmetric part determines rotations, the symmetric part gives dilatations along 3 principal axes. The inhomogeneous term translates the surface.

The connection with Kraus’s evolution of the density matrix over a finite time interval is readily verified in the case of constant coefficients; in such a case, by explicit time integration, one gets the affine [11, 13, 16] map:

\[ \rho' = \sum_i A_i \rho A_i^\dagger \quad \sum_i A_i^\dagger A_i = 1 \]

(7)

which again depends on 12 parameters.

In our problem the hamiltonian is time-dependent: the Poincaré surface still undergoes an affine transformation under a finite time evolution, but the operators $A_i$ are fairly complicate functions of $M(t)$ and $C_i(t)$.

We start by assuming a time-independent matrix $A$ in eq. [1]. The eigenvectors of $D$ identify the dilatation axes of the Poincaré surface. The choice of representation for the hamiltonian part, given by $M$, fixes a second, time-dependent frame.

Everything greatly simplifies if the two frames coincide, i.e. if $D$ is diagonal:

\[ \alpha = \beta = \gamma = 0 \]

The parameters are then reduced from 12 to 9: 3 of them come from the hamiltonian, 3 from decoherence and dissipation, $(\gamma_1, \gamma_2, \gamma_3)$, and the last 3 from the inhomogeneous terms $C_i$.

E.g., in the case of an isotropic thermal bath with average phonon number $\bar{n}$ one has [16]:

\[ \gamma_1 = \gamma_2 = -\gamma (\bar{n} + \frac{1}{2}) \quad \gamma_3 = -\gamma (2\bar{n} + 1) \]
\[ C_1 = C_2 = 0 \quad C_3 = -\gamma \]
4. Unitary evolution

In this section we illustrate the dynamics in the unitary case. The external field is taken, without loss of generality, in the x-z plane: this implies $\Delta' = 0$. We consider an oscillating z-component: $B_z = \omega_0(t)$, and a constant x-component: $B_x = \Delta$.

The evolution can be depicted as a sequence of L-Z crossings and “normal” regimes. We characterize the “normal” regime with the condition $|\omega_0(t)| \gg \Delta$: it is dominated by rotations in the plane $X, Y$, as one can verify by inspection of eq. 5.

One must not expect that the representative on the Poincaré surface retraces its path backwards in coincidence with the external field: in fact the solution is the time-ordered exponential of an operator. This is particularly true when $\omega_0(t)$ is of the order of $\Delta$. On the other hand, as long as the magnetic field $\{\Delta, \omega_0(t)\}$ runs over a line in the plane $\{B_x, B_z\}$, no Berry phase is to be expected.

We take, as an initial condition, the “fully magnetized” configuration $Z = \pm 1$. We have then:

$$
\dot{X} = -\omega_0 Y \quad \dot{Y} = \omega_0 X - \Delta Z \quad \dot{Z} = \Delta Y \quad (8)
$$

$$
\omega_0 = B_0 \cos(\Omega_0 t)
$$

where $\Omega_0$ is the bias frequency.

The Schrödinger equation corresponding to system 8 has the form:

$$
i \dot{a}_1 = \frac{1}{2}(\omega_0 a_1 + \Delta a_2)
$$

$$
i \dot{a}_2 = \frac{1}{2}(-\omega_0 a_2 + \Delta a_1)
$$

where $a_i, (i = 1, 2)$ are the spinor amplitudes.

In the atomic interpretation of the two-level system, $\Delta$ is the interlevel transition amplitude and $\omega_0$ the level spacing.

In the Landau-Zener (L-Z) regime, i.e. close to the level crossing, assumed at $t = 0$, one has: $\omega_0 = \Omega t = B_0 \Omega t$. The asymptotics of the solution, when $\omega_0$ is linear in $t$, is a textbook topic; it can be readily obtained by WKB methods. Let us write the equation for the amplitude $a_2(t)$, in the form:

$$
\frac{d^2}{dt^2} a_2(t) = -W^2(t) \cdot a_2(t) \quad (10)
$$

$$
W(t) = \frac{\Omega t}{2} \sqrt{1 + \left(\frac{\Delta}{\Omega t}\right)^2 - \frac{2i}{t^2 \Omega}}
$$

From the large time behavior of equation 10, we get the semiclassical momentum

$$
p(t) = \frac{\Omega t}{2} + \frac{\nu}{t} \quad \nu = \frac{\Delta^2}{4\Omega}
$$
It is natural to choose the following scattering states: \( \exp\{\pm i\Omega t^2/4\} \cdot (t)^{\pm i\nu} \).

The scattering matrix \( S \) is obtained from the Weber functions, who solve Eq. 10 (see, e.g., [17], and references therein). The procedure is straightforward once one realizes that eq. 10 is the Schrödinger equation for an inverted harmonic oscillator in \( D = 1 \).

The \( S \) matrix identifies a rotation. The branching properties of the solution, characterized by the single parameter \( \nu \), uniquely determine \( S \) and the rotation. Since \( \nu \) is a constant in our system, each crossing produces an identical rotation. Let us label \( S \) with \( \theta, \phi \):

\[
S_{1,1} = \cos(\theta) = \exp\{-\pi \nu\}
\]

\[
S_{1,2} = i \sin(\theta) \cdot \exp\{i\phi\} = \sqrt{\frac{2\pi}{\nu}} \cdot \exp\{-\pi \nu/2 - (i\pi/4)\} \cdot \frac{1}{\Gamma(i\nu)}
\]

\[
S_{2,1} = i \sin(\theta) \cdot \exp\{-i\phi\}
\]

\[
S_{2,2} = S_{1,1}
\]

where \( \Gamma(x) \) is the Gamma function. Clearly \( \theta \) acts on the population \( Z \), and \( \phi \) on the coherences \( X, Y \).

One finds, for the ratio of “in” and “out” populations, \( (T = Z(+\infty)/Z(-\infty)) \):

\[
T = T(\nu) = 2 \cdot \exp\{-2\pi \nu\} - 1.
\]

So far, we discussed the Schrödinger equation. Here we solve the corresponding master equation problem. Notice that, since in going from the spin variables \( a_{1,2} \) to the vector variables \( v_i \) of the density matrix: \( v_i = a_i^* \sigma_i^{l,k} a_k \) \( (i = 1, 2, 3) \), \( (l, k = 1, 2) \), one performs a nonlinear transformation, the new problem is not a straightforward translation of the old one.

Rather than satisfying a second-order order equation as in Eq. 10, each vector component satisfies a third-order equation, so that the connection with the Schrödinger equation is lost.

In spite of that, in the representation of frequencies \( \omega \), the population \( \tilde{Z}(\omega) \) satisfies a Schrödinger equation for an (inverted) harmonic oscillator in \( D = 2 \), with a centrifugal term corresponding to an “angular momentum” \( m = \pm 1 \).

One can develop an \( S \) matrix formalism in this representation, and extract the L-Z rotation from the branching properties of the solution at \( \omega = 0 \): indeed at the level crossing the frequency of the motion inverts its sign. It should be further pointed out that, as long as \( Z \) is quadratic in the spinor amplitudes, its branching behavior is accordingly modified with respect to the spinor case. In Appendix II we give the main steps of the solution.

Before going to numerical results, let us summarize the qualitative features of the motion:

a) in the “normal” regime the representative undergoes uniaxial rotations (precession with time-dependent frequency having an average value of \( \pm 2B_0/\pi \)); b) in the L-Z regime a discrete rotation, involving the population as well as the coherences, occurs; c) in the next “normal” regime the bias \( \omega_0(t) \) has opposite sign with respect to regime (a), so that the sign of precession is inverted in the L-Z region.
Let us consider the following 3 situations: $T \approx 1, 0, -1$.

In the first case we have ($\nu \ll 1$), so that, after crossing, an initially “magnetized” state is preserved, apart from a small correction; in the second case, where the transition probability equals $1/2$, it is turned into a “fully unmagnetized” state; in the third case ($\nu \gg 1$), magnetization reversal occurs.

Fig. 1 is the three-dimensional plot of the representative $v$. The interlevel coupling $\Delta$ is of the order of the frequency $\Omega_0$.

The L-Z crossings can be found in the regions where the trajectory inverts its path. Furthermore, at the crossings the vector $v$ undergoes a discrete rotation $\{\theta, \phi\}$. The vertical angle $\theta$ is determined by the transition probability between the two levels, which goes as $\exp\{-2\pi \cdot \nu\}$: here, where we started with $Z = -1$, one can see that $|Z|$ is reduced accordingly at each crossing.

In Fig. 2, $Z(t)$ is plotted over 10 cycles of the external field. The fast oscillations correspond to the “normal” regime, where $Z$ is on average constant; the “normal” regimes are separated by kinks, produced by the crossings.

Here we have $\theta \approx \pi/3$, as three kinks are needed to reach the complete inversion of $Z$. The population $Z$ (as well as the coherences $X, Y$) undergoes large scale oscillations, following the bias frequency. A planar ($X, Y$) plot would exhibit similar oscillations associated with $\phi$.

One could argue that a zero-average oscillating bias $B_z = \omega_0(t)$ must generate a zero-average $Z(t)$. On the contrary, “single spin magnetization” is possible, with hamiltonian dynamics. Indeed, by operating on the “normal” evolution through $\Omega_0$, we obtained trajectories where $Z(t)$ keeps a fixed sign.

This can be understood as follows. Although the L-Z rotations always act additively on $v$, if the interposed “normal” evolution inverts the planar components, the sequence of the $\theta$ rotations acts on $Z(t)$ alternatingly rather than additively.

Under these conditions if, e.g., one starts with $Z(0) = -1$, and $\theta = \pi/3$, at the first crossing $Z$ is raised at $Z \approx 0.3$, but at the next crossing, it turns back to $Z = -1$. An example is shown in Figs. 3, 4, 5, referring to $Z(t)$, $v(t)$, $Z(B)$ respectively.

In this non-adiabatic regime in general we found strong irreversibility; the “symmetry-breaking” solution instead is almost perfectly reversible. This is made clear in Fig. 5, where practically no hysteretic effects are found.

When the transition probability equals $\frac{1}{2}$, the population, when started at $Z = -1$, turns into a perfectly balanced superposition of the two levels ($Z = 0$) and the vertical angle is: $\theta = \pi/2$. The “in-phase” evolution follows the sequence $Z = -1; 0; 1; 0; -1...$, the “out-of-phase” evolution is given by $Z = -1; 0; -1; 0...$. The latter case again generates a completely reversible process.

At much larger values of the transition probability the magnetization aligns to the bias at each step. The field evolves slowly with respect to the two-level system: we are in the adiabatic regime, and we obtain very small deviations from reversibility in the plots $Z = Z(B)$ (not shown here).
5. Irreversible dynamics: homogeneous case

The simplest non-hermitean generalization of the previous model includes population damping and decoherence. This leads to an homogeneous equation for $v$:

\begin{align}
\dot{X} + \gamma_1 X &= -\omega_0 Y \\
\dot{Y} + \gamma_2 Y &= \omega_0 X - \Delta Z \\
\dot{Z} + \gamma_3 Z &= \Delta Y
\end{align}

(11)

In compact form, we have $\frac{d}{dt} v = \hat{B} \cdot v$. Notice that the isotropic case $\gamma_1 = \gamma_2 = \gamma_3$, apart from a Poincaré sphere with decaying radius, is identical to the unitary case.

We thus consider the general case. The large time asymptotics of the solution of Eq.(1) can be determined from the eigenvalues $p_j(t)$ of the operator $\hat{B}(t)$ [15].

We limit ourselves to few preliminary results, for the sake of simplicity in the uniaxial case: $\gamma_1 = \gamma_2 = \gamma_r; \gamma_3 = \gamma$.

The equation for the right eigenvectors $E_j(t)$ reads:

\[ \hat{B}(t) \cdot E_j(t) = p_j(t) \cdot E_j(t) \]  

(12)

It can be shown [15] that the large time asymptotics is determined by the following fundamental solutions:

\[ v_j(t) \approx \exp\{i \cdot \int_{t_{in}}^t p_j(u) \cdot du\} \cdot E_j(t). \]  

(13)

Since here we have $j = 1, 2, 3$, the eigenvalues can be analytically computed.

It is convenient to shift the variable $p : p \rightarrow y = p + \gamma_r + \delta; [\delta = (\gamma - \gamma_r)/3]$. The eigenvalues are then:

\begin{align}
y_1 &= u + v \\
y_{2,3} &= -\frac{1}{2}[(u + v) \pm i\sqrt{3}(u - v)]
\end{align}

(14)

where $u^3 v^3$ are the roots of the equation:

\begin{align}
t^2 + ft - g^3 &= 0 \\
f &= 2\delta[(\Omega t)^2 + \delta^2 - \frac{1}{2}\Delta^2] \\
g &= \frac{1}{3}[(\Omega t)^2 + \Delta^2 - 3\delta^2]
\end{align}

(15)

In the range of parameters we are interested in, both roots of eq. [15] are real-valued.

We keep terms up to the order $O(1/t^2)$ in the expansion in powers of $t$, and get:

\begin{align}
p_1(t) &\approx -\gamma - 2\gamma_c \frac{1}{(\Omega t)^2} \\
p_{2,3}(t) &\approx -\gamma_r + \gamma_c \frac{1}{(\Omega t)^2} \pm i[\Omega t + \frac{2\nu}{t}] \\
\gamma_c &= \delta(\delta^2 - \frac{1}{2}\Delta^2)
\end{align}

(16)
The first eigenvalue gives the correction to the damping $\gamma$, while $p_{2,3}$ in their real part, give the correction to $\gamma_r$. It is worth noticing that these corrections act on $\gamma$ and $\gamma_r$ with opposite signs: in other words, decoherence is slowed down at the expense of damping, and vice versa, according with the sign of $\gamma_c$.

The imaginary parts of $p_{2,3}(t)$, related with the oscillating behavior and with the branching properties around $t = 0$, are not influenced by decoherence and damping. One verifies that, apart from a factor of 2, which is expected in going from the spinor amplitude to the vector amplitude, the result coincides with the semiclassical momentum $p(t)$, given after eq. [14].

In the example of Fig. 6 we assume pure decoherence in the adiabatic regime: the population $Z$ follows the bias. Notice that indeed $Z$ is damped as expected from the correction to $\gamma$ computed previously (see eq. [16] with $\gamma_c > 0$).

The values of $X$ and $Y$, between crossings, sustain an oscillating $Z$ with an $\langle Z \rangle$ sensitively different from zero.

The symmetry breaking solution, found in the previous section, survives to decoherence, as shown in Fig. 7. Here we have the conditions of Fig. 3, but the decoherence parameters of Fig. 6. One can realize a “magnetized” single spin, by means of an oscillating bias. Here the magnetization is in the direction of the bias field; the situation discussed in ref. [6] is rather different: there the magnetization is orthogonal to the bias and $Z$ relaxes toward the ground state.

When $\gamma_c < 0$, in the adiabatic regime, the dominant effect is that the population decay is enhanced and $Z(t)$ rapidly evolves towards zero.

6. Inhomogeneous case: relaxation from upper to lower level

The incoherent processes in a two-level system include internal transitions (i.e. interlevel transitions mediated by the surroundings).

Here we analyze the effects of incoherent relaxation from the upper to the lower level.

At the L-Z crossings the ground state flips between the two levels, and the inhomogeneous term must change its sign accordingly; we are then led to the inhomogeneous equation:

\[
\begin{align*}
\dot{X} + \gamma_1 X &= -\omega_0 Y \\
\dot{Y} + \gamma_2 Y &= \omega_0 X - \Delta Z \\
\dot{Z} + \gamma_3 (Z + \frac{\omega_0}{|\omega_0|}) &= \Delta Y
\end{align*}
\]

(17)

If one were to choose a sign for the inhomogeneous term in Eq. [17], one would describe a situation in which the system would be forced to decay towards a given level. This is appropriate only provided that $\omega_0$ has a fixed sign.
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The calculations presented in Fig. 8, 9 refer to the adiabatic, strongly damped regime. The population $Z$ starts switching from a “magnetized” state to the opposite one, exactly when the external field changes its sign.

The escape from the instability is markedly different from the relaxation towards the stable ground state (see Fig. 9), but this is not the origin of the hysteretic behavior shown in Fig. 8.

In the approach towards a fully “magnetized” state, the coupling between $Z$ and the coherences $X, Y$ plays a relevant role (see the oscillating branches in the hysteresis cycle). When the bias retraces its path backwards, the system is already in a fully “magnetized” state $Z = \pm 1$, $X = Y = 0$. Only the onset of the instability, as the bias changes its sign, is able to put the system in motion again.

In conclusion, we have two regimes (incoherent $X, Y \approx 0$ and coherent $X, Y \neq 0$ respectively) both compatible with the same value of the bias.

So far we discussed a situation where the period $2\pi/\Omega_0$ is much larger than the decay times of the two-level system, so that the external field can be considered as quasi-static. As the decay time gets longer, the system does not relax fast enough towards the “fully magnetized” state: an hysteretic behavior survives, as shown in Fig. 10.

We conclude this section with a last example: we added the relaxation towards the ground state to the system discussed in Fig. 7; the frequency $\Omega_0$ is comparable with $\Delta$.

In Fig. 11, the fastly oscillating portions refer to the “normal” evolution, and the kinks to the crossings. Notice that the oscillating parts are attracted towards the “fully magnetized” state, which is never reached. The system shows an hysteretic limit cycle (see Fig. 12).

7. Conclusions

We examined the time evolution of a two-level system in the presence of an oscillating external field, both in the unitary case and with decoherence and dissipation. We solved, in this context, the Landau-Zener problem in the density matrix formalism, and showed that, in the frequency representation, the population $\tilde{Z}(\omega)$ satisfies a Schrödinger equation for an inverted harmonic oscillator in $D=2$.

We indicated a procedure allowing to interpret the various dynamical regimes by means of few intuitive rules. We found that it is possible to sustain a magnetization parallel to the bias for the single spin.

We became recently aware of related work [6], where instead the spin is magnetized in the direction orthogonal to the bias; furthermore, while our result holds in the homogeneous case, in Ref. [4] relaxation towards a single level is assumed.

We have also shown that one can explicitly solve the Landau-Zener problem in the non-unitary case, by means of a suitable extension of WKB methods. We stress that in our approach the parameters of the equation are completely arbitrary, so that no “adiabatic elimination” of fast variables is needed [14].
We find that the corrections to $\gamma$ and $\gamma_r$ have opposite sign. The branching properties of the solution are not modified with respect to the unitary case: the scattering matrix is again a function of the single L-Z parameter $\nu$.

When decay from the upper to the lower level is taken into account, we find hysteretic behavior: this effect originates in the coexistence of a fully magnetized state, where the coherences $X, Y$ are strictly zero, and a partly magnetized state, with nonzero coherences. This interpretation holds in the overdamped case; at slower dampings an hysteretic limit cycle survives, related with non-adiabatic effects.

8. Appendix 1. Inequalities following from complete positivity

The conditions for complete positivity of the evolution, when written for matrix $A_{ij}$, are:

$$0 \leq \gamma_1 \leq \gamma_2 + \gamma_3 \quad 0 \leq \gamma_2 \leq \gamma_3 + \gamma_1 \quad 0 \leq \gamma_3 \leq \gamma_1 + \gamma_2$$

together with:

$$4 (\gamma^2 + \frac{1}{4} C_1^2) \leq \gamma_1^2 - (\gamma_2 - \gamma_3)^2$$
$$4 (\beta^2 + \frac{1}{4} C_2^2) \leq \gamma_2^2 - (\gamma_3 - \gamma_1)^2$$
$$4 (\alpha^2 + \frac{1}{4} C_3^2) \leq \gamma_3^2 - (\gamma_1 - \gamma_2)^2$$

$$4 \beta (\alpha \gamma - \frac{1}{4} C_3 C_1) - 2 C_2 (\frac{1}{2} \alpha C_1 + \frac{1}{2} \gamma C_3) \geq (\gamma_1 + \gamma_3 - \gamma_2)(\beta^2 + \frac{1}{4} C_2^2) +$$

$$(\gamma_2 + \gamma_1 - \gamma_3)[\alpha^2 + \frac{1}{4} C_3^2 - \frac{1}{4} \gamma^2 - \frac{1}{4} (\gamma_2 - \gamma_1)^2] + (\gamma_3 + \gamma_2 - \gamma_1)(\gamma^2 + \frac{1}{4} C_1^2)$$

In our problem we further must take into account $\omega_0(t)$, which defines the scale of times, and $\Delta$. Thus $\Delta$ is the single relevant parameter of the model.

9. Appendix II. Solution of the Landau-Zener problem from the master equation

In this Appendix we summarize the main points of the solution of the L-Z problem, as obtained by starting from the master equation; we omit those details that can be easily implemented from the standard solution.

In the non-dissipative case the Landau-Zener problem is written in the form:
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\[ \dot{X} = - (\Omega t) \cdot Y \]
\[ \dot{Y} = (\Omega t) \cdot X - \Delta \cdot Z \]
\[ \dot{Z} = \Delta \cdot Y \] (18)

The variable $Y$ can be eliminated from the third equation, and one obtains:
\[ \ddot{Z} + \Delta^2 \cdot Z = \Delta \Omega t \cdot X \] (19)
\[ \dot{X} = - \frac{\Omega}{\Delta} \cdot \dot{Z} \]

Let us define the new variable $\phi(t) = X(t) + \frac{\Omega}{\Delta} \cdot Z(t)$; it is readily verified, by inspecting the second equation in system (19), that from $\phi(t)$ one can recover the entire solution: $Z(t) = (\Delta/\Omega) \cdot \dot{\phi}(t); X(t) = \phi(t) - t \cdot \dot{\phi}(t)$.

The Fourier transform $\tilde{\phi}(\omega) = \int_{-\infty}^{+\infty} \exp\{-i\omega t\} \cdot \phi(t) \cdot dt$ solves the equation:
\[ \hat{H} \tilde{\phi}(\omega) = 0 \]
\[ \hat{H} = -\frac{\omega^3}{\Omega^2} + \left(\frac{\Delta^2}{\Omega^2} - \frac{\partial^2}{\partial \omega^2}\right)\omega - \frac{\partial}{\partial \omega} \] (20)

Let us write $H$ as:
\[ \hat{H} = \hbar \cdot \omega \]
\[ \hbar = -\frac{\partial^2}{\partial \omega^2} - \frac{1}{\omega} \frac{\partial}{\partial \omega} + \frac{1}{\omega} \frac{\partial}{\partial \omega} - \frac{(\omega)}{\Omega}^2 + \frac{(\Delta)}{\Omega}^2 \] (21)

We find that the function $\chi(\omega) = \omega \cdot \tilde{\phi}(\omega)$, which, apart from a constant factor, is the Fourier transform of the population $Z(t) : (\chi(\omega) = \frac{\Omega}{\Delta} \cdot \tilde{Z}(\omega))$, satisfies the Whittaker equation [18]:
\[ \hat{h} \chi(\omega) = 0. \] (22)

Notice that eq. (22) has the form of a Schrödinger equation for the inverted harmonic oscillator in D=2, with “angular momentum” $m = \pm 1$; (clearly in our case $\omega$ varies over the whole axis).

The equation can be written in the canonical form of the hypergeometric confluent equation (HCE) by letting: $q = \omega^2; \chi(\omega) = \exp\{\frac{i\omega}{2\Omega}\} \cdot (q)^{1/2} \cdot u(q)$.

In terms of the new variable $q : q = (i\Omega) \cdot \xi$, one finally gets, for the function $w(\xi) = u(q)$:
\[ \xi \cdot \frac{d^2}{d\xi^2}w + (2 - \xi) \cdot \frac{d}{d\xi}w - (1 + i\nu) \cdot w = 0 \] (23)
\[ \nu = \frac{\Delta^2}{4\Omega}. \]

Two linearly independent solutions, respectively regular at infinity and around zero, are:
\[ \chi_1(\omega) = \exp\{\frac{i\omega^2}{2\Omega}\} \cdot \omega \cdot \Psi(a, 2, \frac{-i\omega^2}{\Omega}) \]
The Landau-Zener Model with Decoherence: The case \( S = 1/2 \)

\[
\chi_2(\omega) = \exp\left\{ \frac{i\omega^2}{2\Omega} \right\} \cdot \omega \cdot \Phi(a, 2, \frac{-i\omega^2}{\Omega})
\]

\[
a = 1 + i\nu
\]

where \( \Phi, \Psi \) are the hypergeometric confluent functions of first and second type.

In the L-Z problem the large time region is characterized by high frequencies, since there the level spacing always dominates over the interlevel coupling. Hence the solution \( \chi_1(\omega) \), having a well-defined behavior at infinity, is the natural choice in our case.

We consider the behavior of the function \( \Psi(a, c, z) \):

\[
\Psi(a, c, z) \approx (z)^{-a} \cdot [1 + O\left(\frac{1}{z}\right)], \quad (z \gg 1),
\]

and recall that \( \Psi \) satisfies the identity:

\[
\Psi(a, c, z) = (z)^{-1-c} \cdot \Psi(a - c + 1, 2 - c, z).
\]

If one takes the former properties into account, and uses the identity: \( \tilde{\phi}(\omega) = \tilde{\phi}^*(-\omega) \), which follows from \( \phi(t) \) being real, one obtains:

\[
\tilde{\phi}(\omega) = A \exp\left\{ \frac{i\omega^2}{2\Omega} \right\} \cdot \frac{1}{\omega^2} \cdot \Psi(i\nu, 0, \frac{-i\omega^2}{\Omega})
\]

\[
+ A^* \exp\left\{ -\frac{-i\omega^2}{2\Omega} \right\} \cdot \frac{1}{\omega^2} \cdot \Psi(-i\nu, 0, \frac{i\omega^2}{\Omega})
\]

(24)

One recovers the behavior of the population from \( \tilde{Z}(\omega) = i \frac{\Delta}{\Omega} \omega \cdot \tilde{\phi}(\omega) \); we have, as \( \omega \to \infty \), \( \tilde{Z}(\omega) \approx 1/\omega \).

More precisely, apart from constant factors:

\[
\tilde{Z}(\omega) = i \frac{\Delta}{\Omega} \omega \cdot \exp\{-\pi\nu/2\} \cdot \exp\{i\omega^2/(2\Delta)\} \cdot \left(\frac{\omega}{\sqrt{\Omega}}\right)^{-2i\nu} + \exp\{-i\omega^2/(2\Delta)\} \cdot \left(\frac{\omega}{\sqrt{\Omega}}\right)^{2i\nu}
\]

(25)

It is easily verified that the correct transition probabilities can be extracted from the branching properties around \( \omega = 0 \) of the solution \( \tilde{Z}(\omega) \).

We remind that the standard treatment refers to spinor amplitudes, while \( \tilde{Z}(\omega) \) is quadratic in such amplitudes: this explains the factor of 2 in the exponent of \( \omega \).

The coherence \( \tilde{X}(\omega) \), can be found from the identity:

\[
\tilde{X}(\omega) = \tilde{\phi}(\omega) + \frac{d}{d\omega}(\omega\tilde{\phi}(\omega)).
\]

We add the large \( \omega \) behavior of \( \tilde{X}(\omega) \):

\[
\tilde{X}(\omega) \approx \frac{1}{\Omega} \cdot (1 - 2(\frac{\Delta}{\omega})^2) \cdot \exp\{-\pi\nu/2\} \cdot \exp\{i\omega^2/(2\alpha)\} \cdot \left(\frac{\omega}{\sqrt{\Omega}}\right)^{-2i\nu} - \exp\{-i\omega^2/(2\alpha)\} \cdot \left(\frac{\omega}{\sqrt{\Omega}}\right)^{2i\nu}
\]

(26)

In summary, while the Schrödinger equation leads to the inverted harmonic oscillator in \( D=1 \) (Weber equation) in the representation of times, the master equation leads, for \( \tilde{Z}(\omega) \), to the \( D=2 \) inverted harmonic oscillator. Hence, in the representation of frequencies, it is possible to formulate and solve the L-Z problem in terms of the \( S \) matrix.
References

[1] I. Tupitsyn, B. Barbara in: *Magnetoscience - From Molecules to Materials*, Müller, Drillon Eds., Wiley VCH Verlag Gmbh (2000).
[2] V. V. Dobrovitski, M. I. Katsnelson, B. N. Harmon: *Phys. Rev. Lett.* 84, 3458 (2000).
[3] M. Dubé, P. C. E. Stamp: cond-mat/0102156
[4] I. Chiorescu, W. Wernsdorfer, A. Müller, H. Bögg, B. Barbara: *Phys. Rev. Lett.* 84, 15, 3454 (2000).
[5] I. Chiorescu, W. Wernsdorfer, A. Müller, H. Bögg, B. Barbara: *J. Magn. Mat.* 221, 1-2, 103 (2000).
[6] S. Flach, A. M. Miroshnichenko, A. A. Ovchinnikov: quant-ph/0110113.
[7] V. G. Bagrov, J. C. A. Barata, D. M. Gitman, W. F. Wreszinski: *J. Phys.* A35, 175 (2002).
[8] J. C. A. Barata, D. A. Cortez: quant-ph/0202110.
[9] L. D. Landau, E. M. Lifshitz: *Quantum mechanics*, Pergamon Press, Oxford (1967).
[10] C. Zener: *Proc. Roy. Soc. Lond.* A137, 696 (1932).
[11] R. Alicki and K. Lendi. *Quantum Dynamical Semigroups and Applications*. Lect. notes in Phys. 286. Springer-Verlag (1987).
[12] M. B. Ruskai, S. Szarek, E. Werner: cond-mat/0101003; to appear in: *Li. Alg. Appl.*
[13] K. Kraus, *Ann. Physics* 64, 311 (1971).
[14] M. N. Leuenberger, D. Loss: *Phys. Rev.* B61, 12200 (2000).
[15] M. Fedoriuk: *Methodes asymptotiques pour les equations differentielles ordinaires lineaires*, Mir, Moscou, 1987.
[16] G. Strini: *Fortsch. der Phys.* 50, 169 (2002); *Lecture Notes on Quantum Computing* (Unpublished, 2000).
[17] V. L. Pokrovsky, N. A. Sinitsyn: cond-mat/0012303
[18] I. S. Gradsthein, I. W. Rhyzik, *Table of Integrals, Series and Products*. (Academic Press, New York, 1994)
Figure 1. A typical trajectory $v(t), v = X, Y, Z$, starting at $Z = 1$. The “normal” evolution corresponds to the fast uniaxial rotations: here four branches of this sort can be identified. At the crossings the trajectory inverts its path and makes a transition to a new branch. We have $\Delta = 0.01, \Omega_0 = 0.02$; here and in all other figures $B_0 = 1$. 
Figure 2. Time evolution of $Z$ over 10 cycles of the bias field. Three kinks are needed in order to have a complete inversion of the magnetization: hence $\theta = \pi/3$. Here $\Delta = 0.12$, $\Omega_0 = 0.063$. Here and in all the $Z(t)$ plots the scale of time is in arbitrary units.
Figure 3. Time evolution of $Z$ over 10 cycles of the bias field, with $\Delta = 0.12$, $\Omega_0 = 0.0682$. With this choice, at each crossing the vertical rotation changes its sign: the result is an explicit symmetry breaking: $\langle Z(t) \rangle < 0$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{Time evolution of $Z$ over 10 cycles of the bias field, with $\Delta = 0.12$, $\Omega_0 = 0.0682$. With this choice, at each crossing the vertical rotation changes its sign: the result is an explicit symmetry breaking: $\langle Z(t) \rangle < 0$.}
\end{figure}
Figure 4. Trajectory $v(t)$, parameters as in Fig. 3.
Figure 5. Plot of $Z = Z(B)$, from the solution of Fig. 3. Notice that, in spite of being far from the adiabatic regime, the system shows very slight deviations from complete reversibility. These deviations are very sensitive when the system is tuned out of the particular regime displayed in Figs. 3, 4, 5.
Figure 6. Plot of $Z(B)$ for a single cycle of the bias, with initial condition $Z(t = 0) = 1$. The parameters are $\Delta = 0.3$, $\Omega_0 = 0.033$, $\gamma_r = 0.01$, $\gamma = 0$. 
Figure 7. Survival of magnetization in the presence of decoherence: plot of $Z(t)$ over ten periods of the bias, with $\Delta = 0.12$, $\Omega_0 = 0.0682$, $\gamma_r = 0.01$, $\gamma = 0$
Figure 8. Approach to the hysteretic limit cycle in the strongly damped case: $Z(B)$ with $\gamma_r = 0.035, \gamma = 0.07$ and $\Delta = 0.05$, $\Omega_0 = 0.02$. Notice that $Z$ is almost perfectly constant in the fully magnetized branches, where the coherences $X, Y$ are zero. The magnetization reversal starts at the zeros of the bias field.
Figure 9. Plot of the magnetization $Z(t)$ in the same conditions of Fig.6a: the cusps corresponding to the onsets of magnetization reversal separate perfectly identical, but inverted, kinks. The result is a sequence of pulses lacking specular symmetry.
Figure 10. Same as in Fig.6a, but with smaller damping: $\gamma_r = 0.01$, $\gamma = 0.02$. Here the complete magnetization is never reached, because the relaxation towards the ground state has a time scale comparable with the period of the bias. An hysteresis is still obtained; the behavior of $Z(t)$, not displayed here, is again a sequence of asymmetric pulses.
Figure 11. Plot of $Z(t)$ in the non-adiabatic regime; the parameters are as in Fig.5, but now we added the relaxation towards ground state with $\gamma = 0.02$. It is instructive to compare this result with the hamiltonian case of Fig.3b, where we had the same values of $\Delta$ and $\Omega_0$: there $Z$ never changes its sign, here it is attracted towards the lower level. Again each pulse is strongly asymmetric.
Figure 12. Approach to the hysteretic limit cycle of the solution discussed in Fig.8a: one can identify the cusps at the onset of magnetization reversal.