Uniform analytic description of dephasing effects in two-state transitions

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We describe the effect of pure dephasing upon the time-dependent dynamics of two-state quantum systems in the framework of a Lindblad equation for the time evolution of the density matrix. A uniform approximate formula is derived, which modifies the corresponding lossless transition probability by an exponential factor containing the dephasing rate and the interaction parameters. This formula is asymptotically exact in both the diabatic and adiabatic limits; comparison with numerical results shows that it is highly accurate also in the intermediate range. Several two-state models are considered in more detail, including the Landau-Zener, Rosen-Zener, Allen-Eberly, and Demkov-Kunike models, along with several other models, such as a Gaussian model and a Landau-Zener model with a pulsed coupling.

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I. INTRODUCTION

Adiabatic passage is now a widely used tool to control population transfer by external fields [1,2]. This control is at the heart of many applications such as selective photochemistry [3,4] and quantum gates [5–8]. The extension of adiabatic passage to open quantum systems, i.e., to quantum systems coupled to an external environment, is of interest since generally adiabatic processes require relatively long times, where decoherence processes may take place.

Adiabatic passage is based on the following of instantaneous eigenstates (usually dressed by the field in a QED cavity [9], or by a laser field leading to Floquet states [2,10], or by a combination of both [8]). The extension to open systems is made by replacing the Schrödinger equation by a master equation, which describes the effects of the environment. A widely studied class is the linear Lindblad equation, which assumes a Markovian bath with small correlation times [11]. It is associated to a Lindblad generator (LG) which generalizes the Hamiltonian to open systems, and the adiabatic passage is expected to occur along a set of eigenvectors of this LG. There are situations where the LG is not diagonalizable, and Jordan blocks take the role of the eigenvectors [12,13]. However, in most of the current applications the LG are diagonalizable and the appearance of nontrivial Jordan blocks is not generic.

An important question is the description of the adiabatic passage in terms of gaps and avoided crossings of eigenvalues of the LG with associated nonadiabatic couplings. The extension to open systems is not well-established. The aim of this paper is to give such a description using standard two-level models with dephasing (e.g., due to elastic collisions or field fluctuations). We consider the dynamics in the whole range of regimes, i.e., from diabatic to adiabatic. This extends the results of Ref. [14] where such models have been considered in the adiabatic limit, and those of Refs. [15,16] where the effects of dephasing in Landau-Zener transitions is numerically explored. We show in particular that the dynamics evolves in the adiabatic limit along a dark vector connected to the difference of the populations. We derive a uniform approximate formula [Eq. (27)], which adds the effect of dephasing to the known lossless formulas. By comparison with direct numerical simulations we show that this formula gives an excellent approximation both in the adiabatic and in the diabatic limits, and quite good agreement in the intermediate regime.

II. FROM SCHRÖDINGER TO DENSITY MATRIX DYNAMICS

We study the standard resonant (i.e., in the rotating-wave approximation) real Hamiltonian $\mathbf{H}(t)=\Omega(t)\boldsymbol{\sigma}_x/2+\Delta(t)\boldsymbol{\sigma}_z/2$ in the basis $\{|+\rangle, |-\rangle\}$ where $\boldsymbol{\sigma}_j$ are the Pauli matrices, $\Delta(t)$ the detuning from resonance, and $\Omega(t)$ the Rabi frequency (proportional to the field amplitude envelope). The latter is considered positive, whereas the detuning can be positive or negative.

For the purpose of adiabatic passage, it is convenient to consider the Schrödinger equation $i\partial\phi/\partial t=\mathbf{H}(t)\phi$ in the adiabatic basis,

$$i\frac{d\psi}{dt}=[\mathbf{H}_a(t)-\dot{\theta}(t)\boldsymbol{\sigma}_y]\psi, \tag{1}$$

with the diagonal adiabatic Hamiltonian

$$\mathbf{H}_a(t)=\lambda(t)\boldsymbol{\sigma}_z/2, \tag{2}$$

$$\lambda(t)=\sqrt{\Delta^2+\Omega^2}, \tag{3}$$

where

$$\psi=\mathbf{R}^{\dagger}\phi, \tag{4a}$$

$$\mathbf{R}(t)=\begin{bmatrix}\cos[\theta(t)/2] & -\sin[\theta(t)/2]\\ \sin[\theta(t)/2] & \cos[\theta(t)/2]\end{bmatrix}, \tag{4b}$$

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TABLE I. Transition probabilities p_0 in the absence of dephasing and the integral η, Eq. (25b), in some analytically soluble two-state models. Note that the Demkov-Kunike model contains as particular cases the Rosen-Zener model ($B=0$) and the Allen-Eberly model ($\Delta_0=0$).

Model	Parameters	Probabilities
Landau-Zener:	$\Omega(t)=\Omega_0$ $\Delta(t)=t/T^2$	$p_0=1-\exp[-\pi\Omega_0^2T^2/2]$ $\eta=\pi\Gamma\Omega_0 T$
Rosen-Zener:	$\Omega(t)=\Omega_0\,\mathrm{sech}(t/T)$ $\Delta(t)=\Delta_0$	$p_0=\frac{\sin^2\left(\frac{1}{2}\pi\Omega_0 T\right)}{\cosh^2\left(\frac{1}{2}\pi\Delta_0 T\right)}$ $\eta=\frac{2\Gamma\Omega_0 T}{\sqrt{\Omega_0^2+\Delta_0^2}}\ln\frac{\sqrt{\Omega_0^2+\Delta_0^2}+\Omega_0}{\Delta_0}$
Allen-Eberly:	$\Omega(t)=\Omega_0\,\mathrm{sech}(t/T)$ $\Delta(t)=B\tanh(t/T)$	$p_0=1-\frac{\cos^2\left(\frac{1}{2}\pi T\sqrt{\Omega_0^2-B^2}\right)}{\cosh^2\left(\frac{1}{2}\pi BT\right)}$ $\eta=\frac{2\Gamma\Omega_0 T\tan^{-1}\sqrt{B^2/\Omega_0^2-1}}{\sqrt{B^2-\Omega_0^2}}$
Demkov-Kunike:	$\Omega(t)=\Omega_0\,\mathrm{sech}(t/T)$ $\Delta(t)=\Delta_0+B\tanh(t/T)$	$p_0=\frac{\cosh(\pi BT)-\cos(\pi T\sqrt{\Omega_0^2-B^2})}{\cosh(\pi\Delta_0 T)+\cosh(\pi BT)}$ $\eta=\frac{\Gamma\Omega_0 T}{\sqrt{\Omega_0^2+\Delta_0^2-B^2}}\left[\tanh^{-1}\frac{B\Delta_0-B^2+\Omega_0^2}{\Omega_0\sqrt{\Omega_0^2+\Delta_0^2-B^2}}-\tanh^{-1}\frac{B\Delta+B^2-\Omega_0^2}{\Omega_0\sqrt{\Omega_0^2+\Delta_0^2-B^2}}\right]$

$$\tan\theta(t)=\frac{\Omega(t)}{\Delta(t)}\quad[0\leqslant\theta(t)<\pi]. \tag{4c}$$

Adiabatic passage requires $|\dot{\theta}(t)|\ll\lambda(t)$.

There are two important cases of two-state dynamics, characterized by either zero or one crossing of the diabatic energies. The mixing angle $\theta(t)$ has the following limiting values in these two cases:

$$\text{no crossing: } 0 \text{ (respectively } \pi) \xleftarrow{-\infty\leftarrow t} \theta \xrightarrow{t\to\infty} 0 \text{ (respectively } \pi), \tag{5a}$$

$$\text{one crossing: } \pi \xleftarrow{-\infty\leftarrow t} \theta \xrightarrow{t\to\infty} 0, \tag{5b}$$

where we have assumed a nonzero detuning, which changes with time from negative to positive in the level crossing case and is positive (negative) in the no-crossing case. We will study in particular some models that have been widely studied in the literature without decoherence: Landau-Zener, Rosen-Zener, Allen-Eberly, and Demkov-Kunike (see Table I).

The dissipative two-state model can be described in the basis of matrices $\{\mathbf{I}_2,\boldsymbol{\sigma}_x,\boldsymbol{\sigma}_y,\boldsymbol{\sigma}_z\}$. The density matrix can be represented as $\boldsymbol{\rho}(t)=(\mathbf{I}_2+\rho_x\boldsymbol{\sigma}_x+\rho_y\boldsymbol{\sigma}_y+\rho_z\boldsymbol{\sigma}_z)/2$, where the real-valued coherences $\rho_x=\rho_{+-}+\rho_{-+}$ and $\rho_y=i(\rho_{+-}-\rho_{-+})$, and the population inversion $\rho_z=\rho_{++}-\rho_{--}$ (with ρ_{ij} being the density matrix elements) constitute the components of the Bloch vector $\varrho(t)=[\rho_x,\rho_y,\rho_z]$. The total population is conserved during the process, $\rho_{++}+\rho_{--}=1$. In this basis, the dephasing term reads $\boldsymbol{\Gamma}_d=\sqrt{\Gamma/2}\boldsymbol{\sigma}_z$ with Γ the dephasing rate, and the Lindblad equation takes the form of the well-known dissipative Bloch equation [17],

$$\dot{\varrho}(t)=\mathcal{L}(t)\varrho(t), \tag{6}$$

with

$$\mathcal{L}(t)=\begin{bmatrix}-\Gamma & -\Delta(t) & 0\\ \Delta(t) & -\Gamma & -\Omega(t)\\ 0 & \Omega(t) & 0\end{bmatrix}. \tag{7}$$

The mathematical structure of the Bloch equation (6) has the same form as a Schrödinger equation with (non-Hermitian) "Hamiltonian" $\mathcal{H}(t)=i\mathcal{L}(t)$ acting on the three-dimensional space $\mathbb{C}^3$. This Hamiltonian can be decomposed as a sum of a nondissipative term $\mathcal{H}_0(t)$ (the off-diagonal elements) and a dephasing term $\mathcal{H}_d$ (the diagonal elements): $\mathcal{H}(t)=\mathcal{H}_0(t)+\mathcal{H}_d$. We shall find approximate eigenvalues and eigenvectors of this matrix and will analyze the dynamics (diabatic, adiabatic, or intermediate) in terms of those.

The matrix $\mathcal{T}(t)$ that diagonalizes the nondissipative Hamiltonian,

$$\mathcal{T}^{\dagger}(t)\mathcal{H}_0\mathcal{T}(t)=\mathrm{diag}\{\lambda(t),0,-\lambda(t)\}, \tag{8}$$

reads

$$\mathcal{T}(t)=\frac{1}{\sqrt{2}}\begin{bmatrix}-\cos\theta(t) & \sqrt{2}\sin\theta(t) & -\cos\theta(t)\\ -i & 0 & i\\ \sin\theta(t) & \sqrt{2}\cos\theta(t) & \sin\theta(t)\end{bmatrix}, \tag{9}$$

with $\cos\theta(t)=\Delta(t)/\lambda(t)$, $\sin\theta(t)=\Omega(t)/\lambda(t)$.

We now transform the Bloch vector $\varrho(t)$ to the (adiabatic) eigenbasis of $\mathcal{H}_0$,

$$\tilde{\varrho}(t)=\mathcal{T}^{\dagger}(t)\varrho(t), \tag{10}$$

where the tilde hereafter denotes variables in the adiabatic basis. The equation for the nondissipative term reads

$$i\dot{\tilde{\varrho}}(t) = \tilde{\mathcal{H}}_0 e \varrho(t), \tag{11}$$

with $\tilde{\mathcal{H}}_0(t) = \mathcal{T}^\dagger(t)\mathcal{H}_0\mathcal{T}(t) - i\mathcal{T}^\dagger(t)\dot{\mathcal{T}}$, i.e.,

$$\tilde{\mathcal{H}}_0(t) = \begin{bmatrix} \lambda(t) & i\dot{\theta}(t)/\sqrt{2} & 0 \\ -i\dot{\theta}(t)/\sqrt{2} & 0 & -i\dot{\theta}(t)/\sqrt{2} \\ 0 & i\dot{\theta}(t)/\sqrt{2} & -\lambda(t) \end{bmatrix}. \tag{12}$$

If dephasing is included, we have

$$i\dot{\tilde{\varrho}}(t) = [\tilde{\mathcal{H}}_0(t) + \tilde{\mathcal{H}}_d]\tilde{\varrho}(t), \tag{13}$$

with $\tilde{\mathcal{H}}_d = \mathcal{T}^\dagger\mathcal{H}_d\mathcal{T}$, or

$$\tilde{\mathcal{H}}_d = -i\frac{\Gamma}{2}\begin{bmatrix} 1+\cos^2\theta(t) & -\dfrac{\sin 2\theta(t)}{\sqrt{2}} & -\sin^2\theta(t) \\ -\dfrac{\sin 2\theta(t)}{\sqrt{2}} & 2\sin^2\theta(t) & -\dfrac{\sin 2\theta(t)}{\sqrt{2}} \\ -\sin^2\theta(t) & -\dfrac{\sin 2\theta(t)}{\sqrt{2}} & 1+\cos^2\theta(t) \end{bmatrix}. \tag{14}$$

In both cases, the initial state (corresponding to the initial population in $|\pm\rangle$)

$$\varrho(-\infty) = \begin{bmatrix} 0 \\ 0 \\ \pm 1 \end{bmatrix} \tag{15}$$

is connected to the "dark vector"

$$\varrho_D(t) = \begin{bmatrix} \sin\theta(t) \\ 0 \\ \cos\theta(t) \end{bmatrix}, \tag{16a}$$

$$\varrho(-\infty) = \pm\cos\theta(-\infty)\varrho_D(-\infty). \tag{16b}$$

The eigenvector ϱ_D has no y-component and is associated to a null eigenvalue. It is therefore called "dark vector" in analogy to similar properties well-known in the context of adiabatic passage by the stimulated Raman adiabatic (STIRAP) technique [18].

The dynamics of the nondissipative problem in the adiabatic regime occurs along this dark vector, leading to (i) no population transfer in the no-crossing case, or (ii) total population transfer in the level-crossing case. In the nonadiabatic regime, the dark vector is coupled to the two other (bright) eigenvectors, leading to partial transfer of population. In both cases the final population inversion $\rho_{++}-\rho_{--}$ is the final z-component of the dark vector.

III. UNIFORM APPROXIMATION TO THE TRANSITION PROBABILITY

The transition probability in the presence of dephasing can be obtained assuming the following approximations. The coupling between the bright vectors (proportional to $\sin^2\theta$) in $\tilde{\mathcal{H}}_d$ [Eq. (14)] can be neglected in first order since it does not involve the dark vector. Near avoided crossings, the coupling between the dark and bright vectors (proportional to $\sin 2\theta$) in $\tilde{\mathcal{H}}_d$ [Eq. (14)] can be neglected with respect to the diagonal terms of $\tilde{\mathcal{H}}_d$ [Eq. (12)] in the adiabatic regime, and with respect to $\dot{\theta}$ in the diabatic regime. For instance, for the Landau-Zener model (see next section for a detailed description of various models considered here), we have around the avoided crossing (located at $t=0$): $\Gamma\sin 2\theta \sim 2\Gamma t/\Omega_0 T^2$ and $\dot{\theta}\sim -1/\Omega_0 T^2$. In the adiabatic regime ($\Omega_0 T \gg 1$), they are both small. In the diabatic regime ($\Omega_0 T \ll 1$), for which the transition occurs very rapidly around the avoided crossing [19], we have there $|\dot{\theta}| \gg |\Gamma\sin 2\theta|$. For the other models with crossing, similar arguments can be made. This leads to the approximate dissipative operator

$$\tilde{\mathcal{H}}_d \simeq -i\frac{\Gamma}{2}\begin{bmatrix} 1+\cos^2\theta & 0 & 0 \\ 0 & 2\sin^2\theta & 0 \\ 0 & 0 & 1+\cos^2\theta \end{bmatrix}. \tag{17}$$

For the models other than Landau-Zener (see Table I), there is an additional feature in the dynamics: a lifting of quasidegeneracy occurs near the initial and final times [20]. It induces in general initial and final coupling between the dark and bright vectors with final interferences. This feature is not considered here. To prevent the quasidegeneracy, we assume the condition

$$\Delta_0 T, \quad BT \gg 1, \tag{18}$$

where the parameters $\Delta_0 T$, BT are defined in Table I.

We introduce the nondissipative propagator $\mathcal{U}(t,t_i)$, the solution of

$$i\frac{d}{dt}\mathcal{U}(t,t_i) = \mathcal{H}_0(t)\mathcal{U}(t,t_i), \tag{19}$$

and assume that it is known. In the interaction representation, we have to solve

$$i\frac{d}{dt}\tilde{\varrho}' = \tilde{\mathcal{H}}_d'\tilde{\varrho}', \tag{20}$$

with

$$\tilde{\mathcal{H}}_d' = \tilde{\mathcal{U}}^\dagger\tilde{\mathcal{H}}_d\tilde{\mathcal{U}}, \tag{21a}$$

$$\tilde{\varrho}' = \tilde{\mathcal{U}}^\dagger\tilde{\varrho}, \tag{21b}$$

$$\tilde{\mathcal{U}} = \mathcal{T}^\dagger\mathcal{U}\mathcal{T}. \tag{21c}$$

We make the following approximation to solve Eq. (20):

$$[\tilde{\mathcal{U}}, \tilde{\mathcal{H}}_d] = 0, \tag{22}$$

meaning that we decouple the nondissipative propagator from the decohering dynamics. This is justified in the adiabatic limit, when the nondissipative propagator is diagonal. In the diabatic limit, it is still a good approximation near an avoided crossing where the transition is very fast with re-

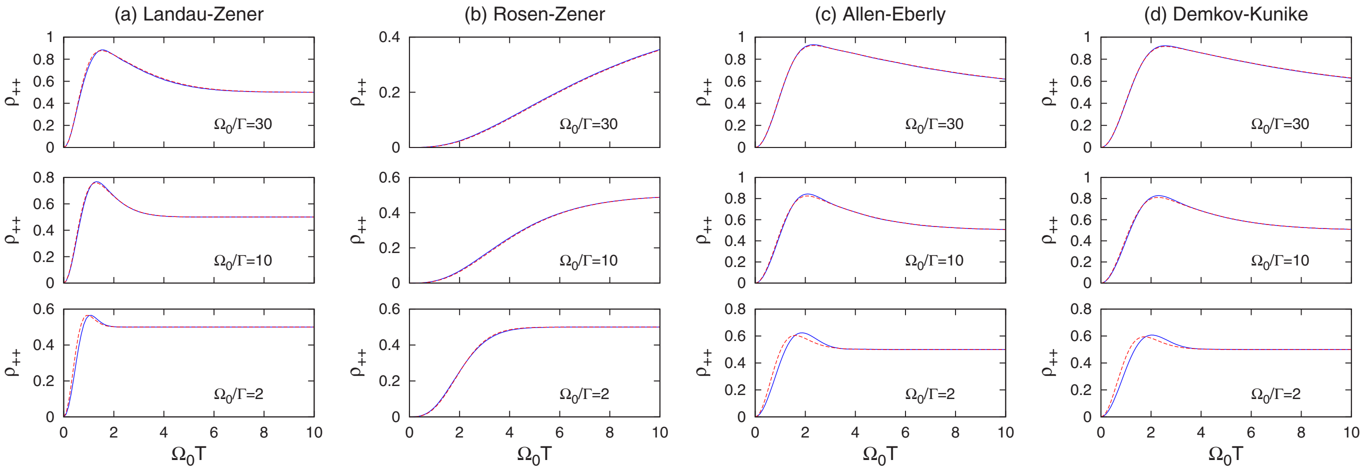

FIG. 1. (Color online) Comparison of the exact numerical solutions (solid lines) with the formula (27) (dotted lines) giving the population ρ_{++} of the upper state at the end of the interaction. Each frame has been computed under the condition (18) for a constant rate Ω_0/Γ, and a constant width T. The parameters used were $\Delta_0 T=3$ for the Rosen-Zener model, $BT=2.5$ for the Allen-Eberly model, and $\Delta_0 T=1$, $BT=3$ for the Demkov-Kunike model.

spect to decohering effects, as shown above, and far from the avoided crossing where the nondissipative propagator is approximately diagonal up to very small corrections.

Below we calculate the solution using the approximations (17) and (22) valid in both adiabatic and diabatic limits, with the condition (18).

With the assumption (22), Eq. (20) has the solution

$$\varrho(t)=\mathcal{U}(t,t_i)\mathcal{T}(t_i)e^{-i\int_{t_i}^{t}\tilde{\mathcal{H}}_d(s)ds}\mathcal{T}^\dagger(t_i)\varrho(t_i). \tag{23}$$

The final population inversion is obtained by taking the z-component of $\varrho(+\infty)$ at the end of the interaction.

In the crossing and no-crossing cases, Eq. (23) reduces to

$$\varrho(\infty)=\mathcal{U}(\infty,-\infty)\begin{bmatrix} e^{-\xi} & 0 & 0 \\ 0 & e^{-\xi} & 0 \\ 0 & 0 & e^{-\eta} \end{bmatrix}\varrho(-\infty), \tag{24}$$

where

$$\xi=\frac{\Gamma}{2}\int_{-\infty}^{\infty}[1+\cos^2\theta(t)]dt, \tag{25a}$$

$$\eta=\Gamma\int_{-\infty}^{\infty}\sin^2\theta(t)dt. \tag{25b}$$

Hence

$$\rho_z(\infty)=e^{-\eta}U_{zz}\rho_z(-\infty)=e^{-\eta}\rho_z^0(\infty). \tag{26}$$

We therefore have in both cases the formula for the transition probability $p\equiv\rho_{++}(\infty)$:

$$p=\frac{1-e^{-\eta}}{2}+e^{-\eta}p_0 \tag{27}$$

with p_0 the transition probability in the absence of dephasing. Obviously, if $\Gamma=0$ (hence $\eta=0$) we have $p=p_0$.

In the adiabatic limit we have for the lossless probability

$$p_0=\begin{cases} 0 & \text{(no crossing)},\\ 1 & \text{(crossing)},\end{cases} \tag{28}$$

and therefore the dephased adiabatic solution is

$$p_a=\begin{cases} \frac{1}{2}(1-e^{-\eta}) & \text{(no crossing)},\\ \frac{1}{2}(1+e^{-\eta}) & \text{(crossing)}.\end{cases} \tag{29}$$

In the diabatic limit we have for both crossing and no-crossing cases $p_0=0$, and hence

$$p_d=\frac{1-e^{-\eta}}{2}. \tag{30}$$

Equation (27) allows us to find the approximate solution in the presence of dephasing for all cases, under the condition (18) for the models other than Landau-Zener.

IV. APPLICATIONS

A. Standard models with decoherence

The transition probabilities for some standard two-state models and the respective integral η, Eq. (25b), are given in Table I. With these values, Eq. (27) provides analytic approximations for the respective two-state models with dephasing included. However, the condition (18) implies some limitations on $\Delta(t)$, making the lossless probability $p_0=0,1$ for every $\Omega_0 T$ in the adiabatic regime.

Numerical simulations are plotted in Fig. 1 for the different models in the case of a strong dephasing ($\Omega_0/\Gamma=2$), a moderate dephasing ($\Omega_0/\Gamma=10$), and a small dephasing ($\Omega_0/\Gamma=30$). The Landau-Zener model is represented in Fig. 1(a); the Rosen-Zener model in Fig. 1(b) for $\Delta_0 T=3$; the Allen-Eberly model in Fig. 1(c) for $BT=2.5$; and the Demkov-Kunike model in Fig. 1(d) for $\Delta_0 T=1$, $BT=3$.

All frames show a very good agreement in the adiabatic regime, since approximation (22) is exactly satisfied. The

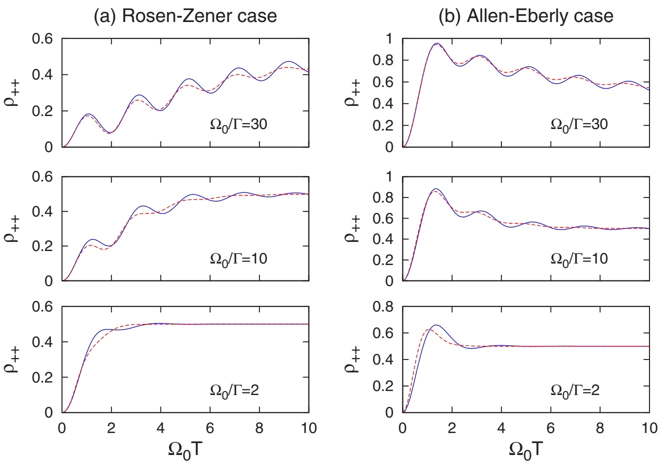

FIG. 2. (Color online) Comparison of the exact numerical solutions (solid lines) with the formula (27) (dotted lines) for $\Delta_0 T=1$ for the Rosen-Zener model and $BT=1$ for the Allen-Eberly model. Each frame has been computed for a constant rate Ω_0/Γ and a constant width T.

results are also good in the other regimes if the dephasing is not to strong, which is the most interesting case in applications. We see that the dephasing does not act in the diabatic limit, while it forces the populations to equality in the adiabatic limit. In particular, the dephasing is responsible for the transition in the Rosen-Zener model, since $p_0=0$ due to Eq. (18).

Figure 2 is the same as Fig. 1 but for $\Delta_0 T=1$ for the Rosen-Zener model and $BT=1$ for the Allen-Eberly model, which reflects the limits of the condition (18). It shows that formula (27) gives, however, a good approximation. In this case the coupling between the dark and the bright vectors cannot be neglected.

B. Generalization to a pulsed Landau-Zener model

The formula (27) can be easily generalized to the case of a linear detuning $\Delta(t)=t/T^2$ and a pulsed coupling $\Omega(t)$. Indeed, if the pulse is large enough, typically $T_p \gg T$, then the avoided crossing can locally be considered as a Landau-Zener process. The transition probability is computed by formula (27), using p_0 given in Table I and η by Eq. (25b). Numerical simulations are shown in Fig. 3 for a strong $(\Omega_0/\Gamma=2)$ and a moderate dephasing $(\Omega_0/\Gamma=10)$ with the following pulses:

$$\text{(a)}\ \Omega(t) = \Omega_0 \exp[-(t/T_p)^2], \tag{31a}$$

$$\text{(b)}\ \Omega(t) = \Omega_0\, \mathrm{sech}(t/T_p), \tag{31b}$$

$$\text{(c)}\ \Omega(t) = \begin{cases} \Omega_0 \cos(t/T_p)^2 & \text{if } -\pi/2 \leqslant t/T_p \leqslant \pi/2 \\ 0 & \text{otherwise,} \end{cases} \tag{31c}$$

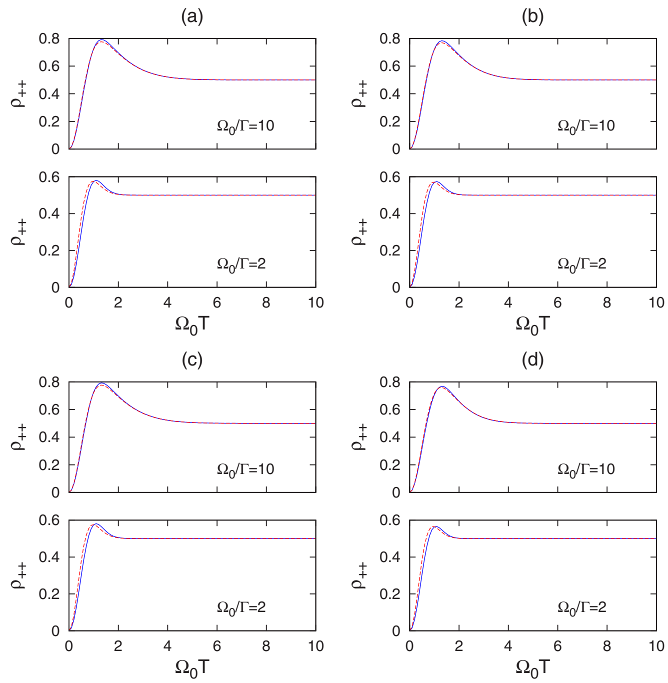

FIG. 3. (Color online) Comparison of the exact numerical solutions (solid lines) with the formula (27) (dotted lines) for a strong and a moderate dephasing. Frame (a) corresponds to a Gaussian pulse, (b) to a hyperbolic secant, (c) to a squared sine, and (d) to a square pulse. Each frame has been computed for a constant rate Ω_0/Γ and a constant width T.

$$\text{(d)}\ \Omega(t) = \begin{cases} \Omega_0 & \text{if } -\pi/2 \leqslant t/T_p \leqslant \pi/2 \\ 0 & \text{otherwise.} \end{cases} \tag{31d}$$

There is a very good agreement between the formula (27) and the simulation in the diabatic and adiabatic regimes, and a quite good one in the intermediate regime.

V. CONCLUSION

We have derived a formula for the transition probability for a class of two-state models subject to dephasing. We have shown that in these cases the dephasing acts as a lossy exponential that multiplies the lossless probability. We have also generalized this formula for models with pulsed coupling and linear detuning. We have shown that this formula gives good results in all the regimes, from diabatic to adiabatic.

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