Adiabaticity condition for non-Hermitian Hamiltonians

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(Received 8 January 2014; published 4 March 2014)

We generalize the concept of population for non-Hermitian systems in different ways and identify the one best suited to characterize adiabaticity. An approximate adiabaticity criterion consistent with this choice is also worked out. Examples are provided for different processes involving two-level atoms with decay.

DOI: 10.1103/PhysRevA.89.033403 PACS number(s): 32.80.Qk, 42.50.−p

I. INTRODUCTION

The adiabatic approximation and adiabatic following are key concepts to study and manipulate quantum systems. For a time-dependent Hamiltonian, the instantaneous eigenvalues and their corresponding eigenstates change with time along time-dependent trajectories. For very slow changes of the control parameters the system will follow closely an eigenstate trajectory up to a phase factor if it is initially in one of the eigenstates. This is the essence of adiabaticity [1] and the adiabatic approximation provides the form of the phase.[1] Adiabaticity is useful for several reasons: The phase factors accompanying adiabatic changes [2] imply many consequences in atomic, molecular, optical, and condensed matter physics; in addition, setting initial and final Hamiltonians as boundary conditions, the details of the parameter paths connecting them are unimportant for the final populations as long as the process is adiabatic. This feature explains the robustness of adiabatic methods to prepare states, the robustness of adiabatic devices such as the atom diode [3,4], or some applications of adiabaticity in quantum information processing [5]. Thus, knowing the conditions that determine the adiabaticity of a given process is generically worthwhile.

For non-Hermitian (NH) systems the usual approximations and criteria [6] are not necessarily valid, so arguments and results that are applicable for Hermitian systems have to be reconsidered and modified [7–23]. We shall review first very briefly some contributions to the study of adiabaticity in NH systems (the selection reflects our interest and is not comprehensive): Dissipative atomic systems motivated the extension of the adiabatic phase and the adiabatic theorem for NH systems [7–9]. A rough estimate of an adiabaticity condition was set by Miniatura *et al*. by analogy with the Hermitian counterpart [8] recognizing the need for further analysis. Nenciu and Rasche [10] distinguished weak and strong non-Hermiticity regimes depending on the ratio between the absolute value of the imaginary parts of the eigenvalues to the slowness parameter. In the weak non-Hermiticity regime (small ratio) a generalization of the adiabatic theorem for nondegenerate eigenvalues is possible. However, in the strong non-Hermiticity regime (large ratio) he pointed out that the usual argument to neglect transitions in the adiabatic limit based on rapidly oscillating exponential phase factors does not apply because the factors blow up exponentially due to the complex energies. An exception is the evolution of the least dissipative state for which all factors decay exponentially. Later, Sun proposed [11], using perturbation theory and integration by parts, an adiabaticity condition similar to the Hermitian one with the real parts of the energies involved in the transition and an exponential factor depending on the imaginary parts. A more sophisticated approach was followed in [13] to set an adiabaticity condition for systems with a discrete and a continuum spectrum subjected to a periodic excitation. These systems are in fact Hermitian, but complex scaling mapped them formally into NH systems discretized by Floquet resonances.

The biorthogonality of the NH Hamiltonian eigenbases implies changes in the definitions of projectors and populations affecting adiabaticity: In [21] different projectors that can be defined in a NH system were exploited (the conventional one, using one eigenstate only, and the one based on biorthogonal resolutions of unity) to compare and discuss different decompositions of the adiabatic phase. Several authors paid attention to the normalization ambiguities in the eigenvectors of NH Hamiltonians [17–19]. This may have dramatic consequences if the adiabaticity condition is defined using ratios of generalized populations. For Hermitian Hamiltonians the adiabaticity conditions imply the conservation of populations for the (time-dependent) instantaneous orthonormal eigenstates [6]. For NH systems, however, the population concept is problematic because of the arbitrariness in the normalization of right and left eigenvectors [17–19] and because of their nonorthogonality and the ensuing nondiagonal contributions to the total state norm. More specifically, Berry and Uzdin stated that "there seems to be no natural normalization" [17] and Leclerc *et al*. in [18] exemplified the difficulties to define adiabaticity based on an arbitrary extension of the population concept to NH systems and proposed a particular definition to avoid them.

For completeness we point out other relevant works, although less directly related to our concern here. In [15,23] the complex time method with Stokes lines was developed to determine transition probabilities in two-level systems including the strong non-Hermiticity regime. In [16,19] methods to design shortcuts to adiabaticity [24–26] were extended to NH systems in the weak non-Hermiticty regime, whereas Torosov *et al*. produced shortcuts to adiabaticity for Hermitian systems using NH Hamiltonians [20]. Finally, several works have been devoted to study the adiabatic flip of the state

[1]A broader concept of adiabaticity applies also to time-independent Hamiltonians with several degrees of freedom, for example, in the Born-Oppenheimer approximation.

and related effects when encircling in parameter space an exceptional point (degeneracy points of the NH Hamiltonian) [8,12,14,17,22,27].

In this paper we provide first different generalizations of the population concept for NH systems and examine their properties. We identify among them the one that is best suited to define an adiabaticity condition for NH systems. A comparison is made with the proposal in [18], which is complementary to ours. We then provide an approximate expression for the adiabaticity condition that improves on the proposal of [11]. Its limitations are also pointed out and examples are presented.

Let us also briefly review the relations that characterize a non-Hermitian system described by a time-dependent Hamiltonian $H(t)$ with N nondegenerate right eigenstates $\{|n(t)\rangle\}$, $n = 1,2,\ldots,N$ [28],

$$H(t)|n(t)\rangle = E_n(t)|n(t)\rangle \tag{1}$$

and biorthogonal partners $\{|\widehat{n}(t)\rangle\}$, which are left eigenstates. Equivalently,

$$H^\dagger(t)|\widehat{n}(t)\rangle = E_n^*(t)|\widehat{n}(t)\rangle, \tag{2}$$

where the asterisk means complex conjugate and the dagger denotes the adjoint operator. They are normalized to satisfy the biorthogonality relation

$$\langle\widehat{n}(t)|m(t)\rangle = \delta_{nm} \tag{3}$$

and the closure relations

$$\sum_n |\widehat{n}(t)\rangle\langle n(t)| = \sum_n |n(t)\rangle\langle\widehat{n}(t)| = 1. \tag{4}$$

The states

$$|\phi_n(t)\rangle = f_n(t)|n(t)\rangle, \tag{5}$$

$$|\widehat{\phi}_n(t)\rangle = \frac{1}{f_n^*(t)}|\widehat{n}(t)\rangle, \tag{6}$$

where $f_n(t) \in \mathbb{C}$ is an arbitrary function [18], constitute also a complete biorthogonal set of eigenstates of $H(t)$. Thus, the freedom to define the eigenvectors of NH Hamiltonians goes beyond the imaginary phase factor ambiguity of Hermitian ones and their ordinary norm $\sqrt{\langle n(t)|n(t)\rangle}$ can be arbitrary. Some restrictions on the $f_n(t)$ apply if the basis is parallel transported, i.e., when $\langle\widehat{n}(t)|\dot{n}(t)\rangle = 0$, where the dot means time derivative. From Eq. (5), taking into account Eq. (3), we find that

$$\langle\widehat{\phi}_n(t)|\dot{\phi}_n(t)\rangle = \dot{f}_n(t)/f_n(t) + \langle\widehat{n}(t)|\dot{n}(t)\rangle. \tag{7}$$

Thus, if the reference basis $\{|n(t)\rangle\}$ is parallel transported and the new basis should be parallel transported too, $f_n(t)$ must be constant. In other words, there is only one parallel transported basis for each set of initial values $f_n(0)$, where we set $t = 0$ as the initial time of the processes. This will be useful later on.

We may expand a state $|\Psi(t)\rangle$ that satisfies the Schrödinger equation

$$i\hbar|\dot{\Psi}(t)\rangle = H(t)|\Psi(t)\rangle \tag{8}$$

as

$$|\Psi(t)\rangle = \sum_n c_n(t)|n(t)\rangle. \tag{9}$$

From Eq. (4), $c_n(t) = \langle\widehat{n}(t)|\Psi(t)\rangle$, but the $|c_n|^2$ are not necessarily bounded by one and their sum does not have to be one either. We may now explore the use of a convenient basis, in particular regarding the definition of adiabaticity.

A state with initial condition $|\Psi(0)\rangle = |n(0)\rangle$ behaves adiabatically if its dynamics is well approximated by $e^{i\beta_n(t)}|n(t)\rangle$. Substituting this form as an ansatz into the Schrödinger equation (8) gives

$$\beta_n(t) = -\frac{1}{\hbar}\int_0^t E_n(t')dt' + i\int_0^t \langle\widehat{n}(t')|\dot{n}(t')\rangle dt'. \tag{10}$$

For a general state, fully adiabatic dynamics (for all modes) would correspond to an evolution of the form

$$|\Psi(t)\rangle = \sum_n g_n(0)|\psi_n(t)\rangle, \tag{11}$$

where

$$g_n(t) := \langle\widehat{\psi}_n(t)|\Psi(t)\rangle, \tag{12}$$

$$|\psi_n(t)\rangle := e^{i\beta_n(t)}|n(t)\rangle, \quad |\widehat{\psi}_n(t)\rangle := e^{i\beta_n^*(t)}|\widehat{n}(t)\rangle. \tag{13}$$

However, the set of states $\{|\psi_n(t)\rangle\}$ and the corresponding biorthogonal partners may be used to expand an arbitrary state, irrespective of its adiabaticity, as

$$|\Psi(t)\rangle = \sum_n g_n(t)|\psi_n(t)\rangle = \sum_n g_n(t)e^{i\beta_n(t)}|n(t)\rangle. \tag{14}$$

Remark 1. While our definition of adiabatic dynamics and the phases in Eq. (10) are quite natural, as they follow from the wave-function ansatz and the Schrödinger equation, an alternative definition and phase based instead on a fidelity criterion also have been proposed [29,30]. The results are not always equivalent [29]. We restrict the present work to the definition given above.

Remark 2. Equation (11) privileges the time zero. There are often physical reasons to do so, in particular when the eigenvectors of $H(0)$ at the preparation time $t = 0$ form an orthonormal basis. A more general view is to associate adiabaticity of a mode n with the approximate invariance of $|g_n(t)|^2$ in Eq. (14) during some time interval that may or may not include the initial time.

II. GENERALIZED POPULATIONS FOR THE EIGENSTATES OF A NON-HERMITIAN HAMILTONIAN

The population of an instantaneous eigenvector $|n(t)\rangle$ of a Hermitian Hamiltonian $H(t)$, $P_n(t) = |\langle n(t)|\Psi(t)\rangle|^2$, may be formally generalized in many different ways for a NH system. Here are some possibilities (we shall frequently omit the time argument t to avoid an overburdened notation):

$$P_{1,n} = |\langle\widehat{n}|\Psi\rangle|^2 = |c_n|^2,$$

$$P_{2,n} = \frac{|\langle\Psi|\widehat{n}\rangle\langle n|\Psi\rangle|}{\sum_n |\langle\Psi|\widehat{n}\rangle\langle n|\Psi\rangle|},$$

$$P_{3,n} = \langle\Psi|\widehat{n}\rangle\langle n|n\rangle\langle\widehat{n}|\Psi\rangle,$$

TABLE I. Properties of different generalized populations [see Eq. (15)].

j	$\sum_n P_{j,n}=1$	$P_{j,n}\leqslant 1$	f independent	Adiabatic invariant
1	no	no	no	no (in general)
2	yes	yes	yes	no
3	no	no	yes	no
4	no	yes	yes	no
5	no	no	no	yes

$$P_{4,n} = \frac{\langle\Psi|\widehat{n}\rangle\langle\widehat{n}|\Psi\rangle}{\langle\widehat{n}|\widehat{n}\rangle\langle\Psi|\Psi\rangle},$$
$$P_{5,n} = |\langle\widehat{\psi}_n|\Psi\rangle|^2 = |g_n|^2. \tag{15}$$

Here $P_{1,n}$ could have in fact different values depending on the criterion for the normalization and phase chosen for the basis functions. A particular choice was proposed in [18], as explained later, and $P_{5,n}$ may be considered a different particular case. Discussions of $P_{j,n}$, for $j = 2,3,4,5$, as generalized populations are lacking, although the amplitudes $g_n(t)$ have been used by several authors to formulate adiabatic approximations for NH systems [11,15,17]. Also the multiplicity relates to the different projectors discussed in [21].

The properties of the generalized populations in (15) are summarized in Table I. They all tend to P_n in the Hermitian limit, when $|\widehat{n}\rangle = |n\rangle$ become orthonormal vectors. This list is not exhaustive. For example, the roles of $|n\rangle$ and $|\widehat{n}\rangle$ may be reversed. We could even consider complex (instead of real) forms. Moreover, some of them add up to one but, since the state norm may change in time for a NH system, it is natural to multiply the generalized populations by the square of the ordinary norm of the state $||\Psi||^2 = \langle\Psi|\Psi\rangle$ so that they sum up to $||\Psi||^2$. The $P_{j,n}$ do not necessarily obey the simple properties of proper populations, such as $\sum_n P_{j,n} = 1$ and $0 \leqslant P_{j,n} \leqslant 1$. Some are f dependent (they change with the change of basis $|n\rangle \to |\phi_n\rangle$ and $|\widehat{n}\rangle \to |\widehat{\phi}_n\rangle$) [see Eqs. (5) and (6)] and others are not. The usefulness of these formal definitions will be determined by their physical content and the intended application. In particular, since our main concern here is the characterization of adiabaticity, the property we should pay attention to is adiabatic invariance. An adiabatic invariant quantity remains constant when the state evolves according to Eq. (11).

The only definition in the group above that is adiabatically invariant independently of the reference basis $\{|n(t)\rangle\}$ chosen is $P_{5,n} = |g_n|^2$, so we shall examine its properties more carefully. The adiabatic invariance of $|g_n|^2$ is guaranteed by construction, but the values of the g_n for an adiabatic evolution, however, will depend on the basis or, in other words, be f dependent, in a mild way. To see why, instead of Eq. (14) we can write the state of the system using a new basis as

$$|\Psi(t)\rangle = \sum_n \widetilde{g}_n(t)\exp\left(-\frac{i}{\hbar}\int_0^t E_n(t')dt' - \int_0^t \langle\widehat{\phi}_n(t')|\dot{\phi}_n(t')\rangle dt'\right)|\phi_n(t)\rangle, \tag{16}$$

where $\widetilde{g}_n(t) = \langle\widehat{\phi}_n(t)|\Psi(t)\rangle$. From Eq. (7), taking into account Eqs. (5) and (6), it follows that

$$\exp\left(-\int_0^t \langle\widehat{\phi}_n(t')|\dot{\phi}_n(t')\rangle dt'\right) = \exp\left(-\int_0^t \langle\widehat{n}(t')|\dot{n}(t')\rangle dt'\right) f_n(0)\Big/ f_n(t)$$

since

$$\exp\left(-\int_0^t \dot{f}_n(t')/f_n(t')dt'\right) = \exp\{\ln[f_n(0)] - \ln[f_n(t)]\}.$$

Thus, comparing Eqs. (16) and (14), we find that $\widetilde{g}_n(t) = g_n(t)/f_n(0)$, i.e., the only difference between the values of these amplitudes for different bases, independently of adiabaticity, is a constant factor $f_n(0)$ that depends on the initial normalization. This residual ambiguity may in fact be suppressed in many processes of physical interest, for which the natural basis at $t = 0$ is orthogonal. This does not necessarily imply that $H(0)$ is Hermitian. For example, in the Landau-Zener or coherent population return processes that we shall discuss in Secs. IV and V for a two-level system, spontaneous decay is always present, even at $t = 0$, so $H(t)$ is never Hermitian. However, before switching the laser on, the bare basis formed by atomic ground and excited states is orthogonal, $\langle n(0)|n'(0)\rangle = 0$ if $n \neq n'$. In principle, it would still be possible to distinguish $|n(0)\rangle$ and $|\widehat{n}(0)\rangle = |n(0)\rangle/\langle n(0)|n(0)\rangle$ from Eq. (3), but the simplest and most useful convention is to set $\langle n(0)|n(0)\rangle = 1$ so that $|\widehat{n}(0)\rangle = |n(0)\rangle$ and $\{|n(0)\rangle\}$ becomes an ordinary orthonormalized basis at the initial instant of time. Then the $P_{5,n}(0) = |g_n(0)|^2$ become ordinary populations $P_n(0)$. Hereafter we shall limit the discussion to this type of system and convention, in which a natural normalization [17] does exist. From Eqs. (5) and (6), the only allowed $f_n(0)$ to satisfy the orthonormalization condition $\langle n(0)|n'(0)\rangle = \delta_{n,n'}$ are of modulus one, so $|\widetilde{g}_n(t)|^2 = |g_n(t)|^2$, even if the system does not follow adiabatic dynamics. For nonadiabatic dynamics, the $|g_n(t)|^2$ are not bounded by one and their sum over n may be anything. However, if $\sum_n |g_n(0)|^2 = 1$, the sum will still be one as long as the evolution remains adiabatic for all states, $\sum_n |g_n(t)|^2 = 1$. This means that 1 becomes the relevant scale to identify adiabaticity or its absence in each of the $|g_n(t)|^2$ terms. For a state that begins like $|\Psi(0)\rangle = |m(0)\rangle$, with $|g_m(0)|^2 = 1$, adiabatic dynamics implies $|g_m(t)|^2 \approx 1$, whereas for $n \neq m$, with $|g_n(0)|^2 = 0$, adiabaticity implies $|g_n(t)|^2 \ll 1$.

We may consider instead of Eqs. (14) and (16) the expansions

$$|\Psi(t)\rangle = \sum_n d_n(t)\exp\left(-\int_0^t \langle\widehat{n}(t')|\dot{n}(t')\rangle dt'\right)|n(t)\rangle, \tag{17}$$

$$|\Psi(t)\rangle = \sum_n \widetilde{d}_n(t)\exp\left(-\int_0^t \langle\widehat{\phi}_n(t')|\dot{\phi}_n(t')\rangle dt'\right)|\phi_n(t)\rangle \tag{18}$$

(see [18]) without an explicit dynamical factor. [If the basis is parallel transported $d_n(t) = c_n(t)$.] The coefficients $d_n(t)$ are also weakly dependent on a basis change, i.e., they obey $\widetilde{d}_n(t) = d_n(t)/f_n(0)$. However, for NH systems they may suffer

strong exponential variations even for adiabatic dynamics, as

$$d_n(t) = g_n(t) \exp\left(\frac{-i}{\hbar}\int_0^t E_n(t')dt'\right), \tag{19}$$

and the E_n are generally complex. As a consequence, the ratios $|d_n(t)|^2/|d_{n'}(t)|^2$, for $n \neq n'$, change dramatically due to different exponential dynamical factors even when the two implied states behave adiabatically. In any case the d_n coefficients may be physically very relevant. If a parallel-transported basis $\{|n(t)\rangle\}$ becomes orthonormalized again at the final process time t_f, the $|d_n(t_f)|^2$ would directly give actual populations, unlike the $|g_n(t_f)|^2$, generally affected by suppressing or enhancing dynamical exponentials. This is important because nonadiabatic excitations revealed in the $\{|\psi_n\rangle\}$ basis by a large $|g_n(t_f)|^2$ value might actually be irrelevant in practice if the corresponding $|d_n(t_f)|^2$ turns out to be negligible. In general it is advisable to analyze a given process simultaneously in different bases.

III. APPROXIMATE ADIABATICITY CONDITION FOR NON-HERMITIAN HAMILTONIANS

In the previous section we discussed a general exact criterion of adiabaticity that requires calculating the $|g_n|^2$, and thus the exact dynamics, to be applied. Here we shall work out a simpler approximate criterion. As in [16,19], assuming that the general state of the system is given by Eq. (14), parallel transported eigenstates so that $\langle\widehat{n}|\dot{n}\rangle = 0$, and inserting Eq. (14) into the Schrödinger equation (8), we get

$$\dot{g}_n(t) = -\sum_{k\neq n} e^{iW_{nk}(t)}\langle\widehat{n}(t)|\dot{k}(t)\rangle g_k(t), \tag{20}$$

where $W_{nk}(t) = \int_0^t \omega_{nk}(t')dt'$ and $\omega_{nk}(t) := [E_n(t) - E_k(t)]/\hbar$. (Note that all exponentials decay if n corresponds to the least dissipative state at all times [10].) Integrating this formally gives

$$g_n(t) - g_n(0) = -\sum_{k\neq n}\int_0^t e^{iW_{nk}(t')}\langle\widehat{n}(t')|\dot{k}(t')\rangle g_k(t')dt'.$$

We now apply perturbation theory. Assuming that the system is initially in $|m(0)\rangle$ and approximating the coefficients $g_k(t)$ inside the integral as $g_k(t) = \delta_{km}$, one finds to first order, for $n \neq m$,

$$g_n(t) = -\int_0^t \langle\widehat{n}(t')|\dot{m}(t')\rangle e^{iW_{nm}(t')}dt', \tag{21}$$

which should satisfy $|g_n(t)| \ll 1$ for an adiabatic evolution. Rewriting Eq. (21) as $g_n(t) = -\int_0^t u_n dv_n$, with

$$\begin{aligned} u_n &= \frac{\langle\widehat{n}(t')|\dot{m}(t')\rangle}{i\omega_{nm}(t')}, \\ dv_n &= i\omega_{nm}(t')e^{iW_{nm}(t')}dt', \end{aligned} \tag{22}$$

and integrating by parts, we find

$$g_n(t) = -\frac{\langle\widehat{n}(t')|\dot{m}(t')\rangle}{i\omega_{nm}(t')}e^{iW_{nm}(t')}\Big|_0^t + \int_0^t v_n du_n. \tag{23}$$

Neglecting the integral term in Eq. (23), which, as shown in Appendix A, involves higher inverse powers of ω_{nm} and the (generally small) contribution at $t = 0$, we get from $|g_n(t)| \ll 1$ the approximate adiabaticity condition

$$|(uv)_n(t)| = \frac{|\langle\widehat{n}(t)|\dot{m}(t)\rangle|}{|\omega_{nm}(t)|}e^{-\mathrm{Im}[W_{nm}(t)]} \ll 1 \tag{24}$$

for $n \neq m$. For $n = m$ a second-order integral may be written, but it does not lead to a simple expression by integration by parts. The fact that the condition (24) is limited to $n \neq m$ is quite harmless for Hermitian systems because of the conservation of total probability and the orthogonality of states. In a NH system it is a more serious limitation, as we cannot deduce from it the adiabaticity or otherwise of the initially occupied state. The criterion (24) is a natural generalization of the usual Hermitian criterion and it outperforms other approximations based on partitions of Eq. (21) alternative to Eq. (22), such as [11]

$$\begin{aligned} u_n' &= \frac{\langle\widehat{n}(t')|\dot{m}(t')\rangle e^{-\mathrm{Im}[W_{nm}(t')]}}{i\ \mathrm{Re}[\omega_{nm}(t')]}, \\ dv_n' &= i\ \mathrm{Re}[\omega_{nm}(t')]e^{i\ \mathrm{Re}[W_{nm}(t')]}dt'. \end{aligned} \tag{25}$$

Similarly we could try

$$\begin{aligned} u_n'' &= \frac{\langle\widehat{n}(t')|\dot{m}(t')\rangle e^{i\ \mathrm{Re}[W_{nm}(t')]}}{-\mathrm{Im}[\omega_{nm}(t')]}, \\ dv_n'' &= -\mathrm{Im}[\omega_{nm}(t')]e^{-\mathrm{Im}[W_{nm}(t')]}dt'. \end{aligned} \tag{26}$$

These partitions lead to conditions similar to Eq. (24), but with $|\mathrm{Re}(\omega_{nm})|$ [11], for Eq. (25), and $|\mathrm{Im}(\omega_{nm})|$, for Eq. (26), in the denominator. In processes such as a Landau-Zener transition for a two-level atom discussed later, the real or the imaginary parts of the energies may become equal for some t, but $|\omega_{nm}|$ is always different from zero as long as fully degenerate points (with equal eigenvalues) are not crossed.

IV. MODELS: LANDAU-ZENER AND COHERENT POPULATION RETURN PROCESSES FOR A TWO-LEVEL ATOM

We shall exemplify the previous analysis with two types of adiabatic processes of physical interest for a decaying two-level atom: a Landau-Zener (LZ) protocol with constant laser intensity, which in the appropriate parameter range produces population inversion, and coherent population return (CPR) with constant laser detuning and Gaussian Rabi frequency, a useful process to suppress power broadening [31]. We assume for simplicity that a Hamiltonian description, rather than a master equation, is enough for the trapped atom [16,32,33]. This happens, for example, when the decayed atom escapes from the trap by recoil. We shall also assume a semiclassical treatment of the interaction between the electric field and the atom, as well as a constant decay rate Γ, the inverse lifetime, from the excited state to the ground state.

Applying the electric dipole approximation, a laser-adapted interaction picture, and the rotating-wave approximation, the Hamiltonian, disregarding atomic motion, is [34]

$$H_{a0}(t) = \frac{\hbar}{2}\begin{pmatrix} -\Delta(t) & \Omega_R(\Omega) \\ t_R(t) & \Delta(t) - i\Gamma \end{pmatrix} \tag{27}$$

in the bare basis $|\text{g.s.}\rangle = \binom{1}{0}$ and $|\text{e.s.}\rangle = \binom{0}{1}$ of the atom. The norm of the general state $|\Psi(t)\rangle$ decreases due to spontaneous decay. The detuning is defined as $\Delta(t) = \omega_0 - \omega(t)$, where $\omega(t)/2\pi$ is the instantaneous field frequency and $\omega_0/2\pi$ the transition frequency. The (real) Rabi frequency $\Omega_R(t)$ in general also depends on time. The eigenvalues of this Hamiltonian are

$$E_\pm(t) = \frac{\hbar}{4}\left\{-i\Gamma \pm \sqrt{-[\Gamma + 2i\,\Delta(t)]^2 + 4\Omega_R^2(t)}\right\} \tag{28}$$

and the right eigenstates, which play the role of $\{|n(t)\rangle\}$ here, are

$$\begin{aligned} |+(t)\rangle &= \sin\left(\frac{\alpha}{2}\right)|\text{g.s.}\rangle + \cos\left(\frac{\alpha}{2}\right)|\text{e.s.}\rangle, \\ |-(t)\rangle &= \cos\left(\frac{\alpha}{2}\right)|\text{g.s.}\rangle - \sin\left(\frac{\alpha}{2}\right)|\text{e.s.}\rangle, \end{aligned} \tag{29}$$

where the mixing angle $\alpha = \alpha(t)$ is complex and defined by

$$\tan[\alpha(t)] = \frac{\Omega_R(t)}{\Delta(t) - i\Gamma/2} \tag{30}$$

as $\alpha = \arctan(x) = i[\ln(1 - ix) - \ln(1 + ix)]/2$, with

$$x(t) = \frac{\Omega_R(t)}{\Delta(t) - i\Gamma/2}. \tag{31}$$

The adjoint of $H_{a0}(t)$ is

$$H_{a0}^\dagger(t) = \frac{\hbar}{2}\begin{pmatrix} -\Delta(t) & \Omega_R(t) \\ \Omega_R(t) & \Delta(t) + i\Gamma \end{pmatrix}, \tag{32}$$

with eigenvalues $E_\pm^*(t)$ and right eigenstates

$$\begin{aligned} |\widehat{+}(t)\rangle &= \sin\left(\frac{\alpha^*}{2}\right)|\text{g.s.}\rangle + \cos\left(\frac{\alpha^*}{2}\right)|\text{e.s.}\rangle, \\ |\widehat{-}(t)\rangle &= \cos\left(\frac{\alpha^*}{2}\right)|\text{g.s.}\rangle - \sin\left(\frac{\alpha^*}{2}\right)|\text{e.s.}\rangle. \end{aligned} \tag{33}$$

The coefficients are complex conjugate of those in Eq. (29) because $H_{a0}(t)$ is equal to its transpose [28]. For later use we calculate the matrix elements

$$\langle\widehat{\pm}(t)|\partial_t|\pm(t)\rangle = 0, \tag{34}$$

$$\langle\widehat{\mp}(t)|\partial_t|\pm(t)\rangle = \pm\frac{\dot\alpha}{2}, \tag{35}$$

where

$$\dot\alpha(t) = \frac{\dot\Omega_R(t)[\Delta(t) - i\Gamma/2] - \Omega_R(t)\dot\Delta(t)}{[\Delta(t) - i\Gamma/2]^2 + \Omega_R^2(t)}. \tag{36}$$

Equation (34) shows that the states $|+(t)\rangle$ and $|-(t)\rangle$ are parallel transported. To impose the continuity of the eigenvalues and eigenvectors throughout the process and the correct matching of their $\pm$ labels we have to choose the branches of the square root in Eq. (28) and of the arctan (x). For each protocol $\Delta(t)$ and $\Omega_R(t)$ are specified and we have to analyze the behavior of the radicand in Eq. (28),

$$z(t) = -[\Gamma + 2i\,\Delta(t)]^2 + 4\Omega_R^2(t). \tag{37}$$

Here $z(t)$ is in polar form $z = Re^{i\gamma}$, with modulus $R = |\sqrt{\text{Re}(z)^2 + \text{Im}(z)^2}|$ and argument γ, where $\text{Re}(z) = 4\Delta^2(t) + 4\Omega_R^2(t) - \Gamma^2$ and $\text{Im}(z) = -4\Delta(t)\Gamma$.

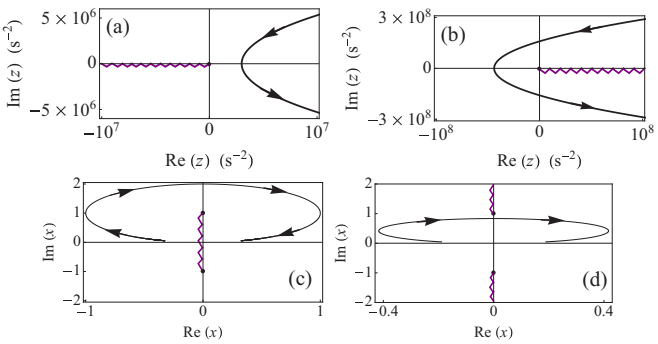

FIG. 1. (Color online) Landau-Zener processes: branch cuts and representative trajectories in the complex z and x planes [see Eqs. (37) and (31)]. For (a) and (c) $\Gamma < 2\Omega_0$ ($\Gamma = 2\pi \times 0.159$ kHz, $\Omega_0 = 2\pi \times 0.159$ kHz, $b = 2 \times 10^6$ s^{-2}, and $t_f = 3$ ms); for (b) and (d) $\Gamma > 2\Omega_0$ ($\Gamma = 2\pi \times 1.910$ kHz, $\Omega_0 = 2\pi \times 0.796$ kHz, $b = 50 \times 10^6$ s^{-2}, and $t_f = 1$ ms). The branch cut in (a), just below the negative real axis, is chosen so that $-\pi < \gamma \leqslant \pi$ and in (b), just below the positive real axis, is chosen so that $0 \leqslant \gamma < 2\pi$.

The first process we consider is the Landau-Zener protocol, with linear detuning and constant Rabi frequency

$$\Delta_{LZ}(t) = b(t - t_f/2), \tag{38}$$

$$\Omega_{R,LZ}(t) = \Omega_0, \tag{39}$$

where t_f is the final time of the process, $b > 0$ is the constant chirp, and Ω_0 is the constant Rabi frequency. Two regimes can be distinguished for this protocol depending on whether $\Gamma < 2\Omega_0$ or $\Gamma > 2\Omega_0$ (a degeneracy exists at $t = t_f/2$ if $\Gamma = 2\Omega_0$).

(i) When $\Gamma < 2\Omega_0$, then $\text{Re}(z) > 0$. A representative trajectory of z in the complex z plane is shown in Fig. 1(a). We choose the branch cut of the square root just below the negative real axis so that $-\pi < \gamma \leqslant \pi$. The imaginary parts of both energies cross each other at $t = t_f/2$, where $\text{Im}[E_+(t_f/2)] = \text{Im}[E_-(t_f/2)] = -i\hbar\Gamma/4$ and the real parts have an avoided crossing at this instant of time [see Figs. 2(a) and 2(b)]. With this branch election $\text{Im}[E_+(t)] > \text{Im}[E_-(t)]$ when $t < t_f/2$ and $\text{Im}[E_-(t)] > \text{Im}[E_+(t)]$ when $t > t_f/2$, which implies that the least dissipative state changes from $|+(t)\rangle$ when $t < t_f/2$ to $|-(t)\rangle$ when $t > t_f/2$. The initial detuning is negative [see Eq. (38)] and the trajectory of x in the complex plane is depicted in Fig. 1(c), so we choose for continuity the arctan (x) branch cut in that figure. Note the inversions $|+(0)\rangle \approx |\text{g.s.}\rangle \to |+(t_f)\rangle \approx |\text{e.s.}\rangle$ and $|-(0)\rangle \approx -|\text{e.s.}\rangle \to |-(t_f)\rangle \approx |\text{g.s.}\rangle$ as $\alpha(0) \approx \pi \to \alpha(t_f) \approx 0$. This model describes rapid adiabatic passage by a LZ protocol in the presence of decay.

(ii) When $\Gamma > 2\Omega_0$, z crosses the negative real axis as shown in Fig. 1 (b) and we choose the branch cut for the square root just below the positive real axis so that $0 \leqslant \gamma < 2\pi$. Now the real parts of $E_\pm(t)$ cross at $t = t_f/2$, where $\text{Re}[E_+(t_f/2)] = \text{Re}[E_-(t_f/2)] = 0$ and $\text{Im}[E_+(t)] > \text{Im}[E_-(t)]$ [see Figs. 2(c) and 2(d)]. Thus, $|+(t)\rangle$ is the least dissipative state for the whole process. The form of the x trajectory is depicted in Fig. 1(d). We choose the branch cuts as depicted in the figure to ensure continuity and add π to

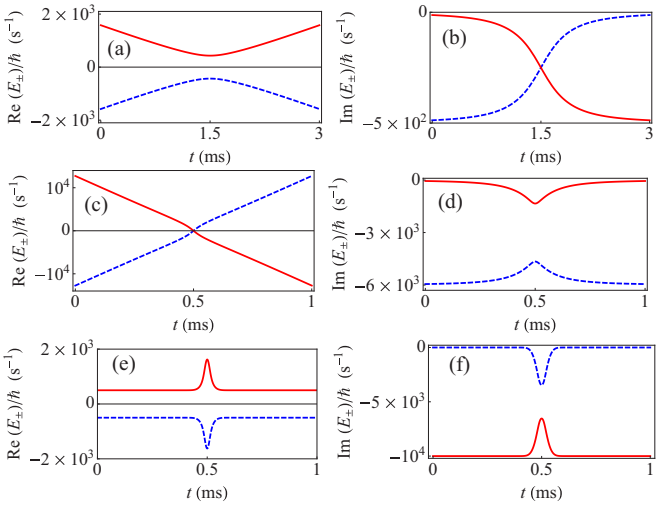

FIG. 2. (Color online) Real and imaginary parts of the energies for a Landau-Zener and CPR processes: (a) and (b) LZ, $\Gamma < 2\Omega_0$; (c) and (d) LZ, $\Gamma > 2\Omega_0$; (e) and (f) CPR. The red solid line denotes E_+ and the blue dashed line E_-. The parameters are the same as in Fig. 1 for LZ and $\Gamma = 2\pi \times 3.183$ kHz, $\Omega_{\max} = 2\pi \times 1.592$ kHz, $a = 4 \times 10^8$ s^{-2}, $\Delta_0 = 2\pi \times 0.159$ kHz, and $t_f = 1$ ms for CPR.

define α so as to match the $\pm$ labeling of eigenvectors and eigenvalues. Here α evolves from $\alpha(0) \approx \pi$ to $\alpha(t_f) \approx \pi$ and the eigenvectors are not inverted: $|+(0)\rangle \approx |+(t_f)\rangle \approx |\text{g.s.}\rangle$ and $|-(0)\rangle \approx |-(t_f)\rangle \approx -|\text{e.s.}\rangle$.

The second type of process we consider is CPR [31] with constant detuning $\Delta_0 > 0$ and a Rabi frequency given by a Gaussian function

$$\Delta_{CPR}(t) = \Delta_0, \tag{40}$$

$$\Omega_{R,CPR}(t) = \Omega_{\max} e^{[-a(t-t_f/2)^2]}, \tag{41}$$

where $\Omega_{\max}$ and a are constants. For this process z has a constant imaginary part $\text{Im}(z) = -4\Gamma\Delta_0$. Thus, $z(t)$ never crosses the real axis and we may choose the branch cut along (just below) the negative part of this axis, as shown in Fig. 3(a). Then, $|-\rangle$ is the least dissipative state throughout. The trajectory of x moves back and forth in the first quadrant, so the branch cuts are chosen as depicted in Fig. 3(b), without adding π to define α. Now $\alpha(0) \approx \alpha(t_f) \approx 0$, $|+(0)\rangle \approx |+(t_f)\rangle \approx |\text{e.s.}\rangle$, and $|-(0)\rangle \approx |-(t_f)\rangle \approx |\text{g.s.}\rangle$. The eigenenergies behave as in Figs. 2(e) and 2(f).

V. NUMERICAL EXAMPLES

In this section we shall provide, based on the two-level model, some examples to illustrate different features of adiabaticity for NH systems, defined in terms of the amplitudes $g_n(t)$. We shall mostly pay attention to properties that differ from the ones of Hermitian systems.

Figure 4 compares, for a CPR process, the rather different behavior of $|g_\pm|$ [Figs. 4(a) and 4(c)] and $|d_\pm|$ [Figs. 4(b) and 4(d)]. Here, from Eq. (34), $d_\pm(t) = c_\pm(t)$. In Figs. 4(a) and 4(b) the initial state is the ground state, which evolves adiabatically as the least dissipative state. Figure 4(a) for $|g_\pm|$ shows an interesting feature of NH systems, namely, that one state may

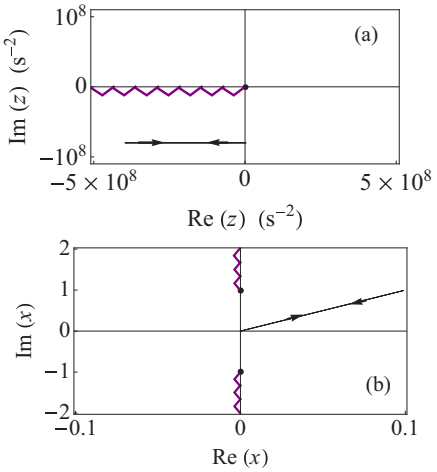

FIG. 3. (Color online) The CPR process: branch cuts and representative trajectories in the complex (a) z and (b) x planes [see Eqs. (37) and (31)], with the parameters the same as in Fig. 2.

remain adiabatic, whereas the other one does not. This is not reflected as clearly in Fig. 4(b) for $|d_\pm|$. Figures 4(c) and 4(d) correspond to the atom starting in the most dissipative state. Figure 4(c) for $|g_\pm|$ shows that for the time considered both states remain perfectly adiabatic. However, the $|d_+|$ coefficient decays strongly because of spontaneous decay [see Fig. 4(d)], so a ratio $|d_-|/|d_+|$ is not a faithful indicator of adiabaticity. Nevertheless, as pointed out earlier, these coefficients are actually quite relevant, in particular at t_f, because here the states $|\pm(t_f)\rangle$ become orthonormalized and coincide with the bare basis of excited and ground atomic states.

On a different thread, note that in the examples of Figs. 4(a) and 4(c), $|(uv)_\pm|$ [see Eqs. (22)–(24)], are very good approximations to $|g_\pm|$ for the initially unoccupied states [the subscript in $|(uv)_\pm|$ specifies which amplitude $|g_\pm|$ is approximated].

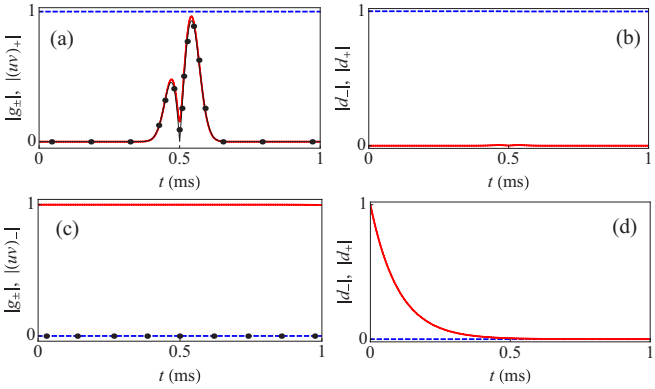

FIG. 4. (Color online) Plot of $|g_\pm|$, $|d_\pm|$, and $|(uv)_\pm|$ for a CPR process: (a) and (b) $|\Psi(0)\rangle = |\text{g.s.}\rangle = |-(0)\rangle$ (least dissipative) and (c) and (d) $|\Psi(0)\rangle = |\text{e.s.}\rangle = |+(0)\rangle$ (most dissipative). The red solid line is for $|g_+|$ and $|d_+|$ and the blue dashed line for $|g_-|$ and $|d_-|$. The black dots are the approximation $|(uv)_\pm|$ for the state that is not populated initially. The parameters are $\Gamma = 2\pi \times 3.183$ kHz, $\Omega_{\max} = 2\pi \times 3.183$ kHz, $a = 4 \times 10^8$ s^{-2}, $\Delta_0 = 2\pi \times 31.831$ kHz, and $t_f = 1$ ms.

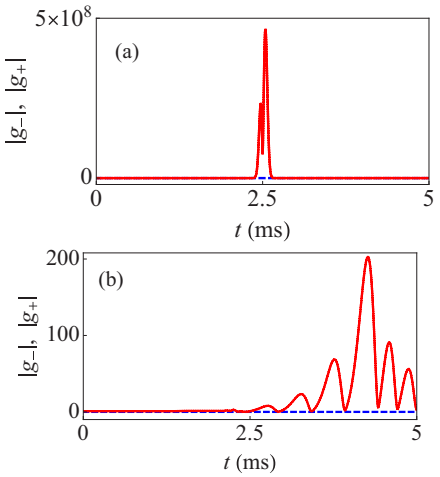

FIG. 5. (Color online) Plot of $|g_+|$ (red solid line) and $|g_-|$ (blue dashed line) for a CPR process when (a) $|\Psi(0)\rangle = |\text{g.s.}\rangle = |-(0)\rangle$ and (b) $|\Psi(0)\rangle = |\text{e.s.}\rangle = |+(0)\rangle$ for the parameters $\Gamma = 2\pi \times 3.183$ kHz, $\Omega_{\max} = 2\pi \times 3.183$ kHz, $a = 4 \times 10^8$ s^{-2}, $\Delta_0 = 2\pi \times 31.831$ kHz, and $t_f = 5$ ms.

Figure 5 is about a CPR process with a final time five times larger than in the previous figure. Contrary to Hermitian systems, longer process times may actually spoil adiabaticity for NH systems. Figure 5(b) shows [compare to Fig. 4(c)] that when the system starts in the most dissipative state $|+\rangle$, it does not remain adiabatic if the time is large enough. Contrast this also to Fig. 5(a), where the system starts and stays adiabatic in the least dissipative state $|-\rangle$ while $|+\rangle$ is excited.

The approximations $|(uv)_\pm|$ in Eq. (24) are depicted in Fig. 6 on a logarithmic scale for Landau-Zener processes with decay for $\Gamma < 2\Omega_0$ [Figs. 6(a) and 6(c)] and $\Gamma > 2\Omega_0$ [Figs. 6(b) and 6(d)]. In general, the criterion $|(uv)_\pm| \ll 1$ avoids the gross pitfalls of simpler choices at crossings of the real and imaginary parts of the energies [see Eqs. (25) and (26)] as long as a fully degenerate point (when both real and imaginary parts are equal) is not crossed.

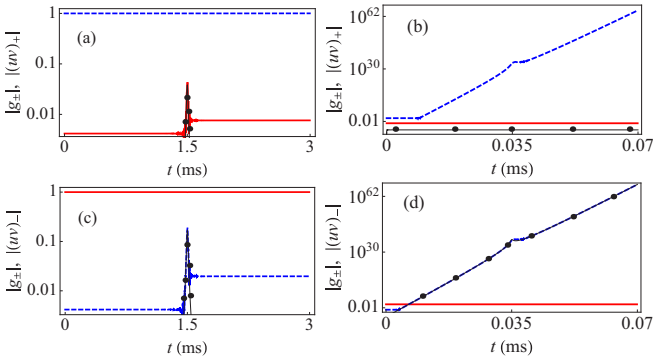

FIG. 6. (Color online) Plot of $|(uv)_\pm|$ and $|g_\pm|$ for two Landau-Zener processes. The red solid line denotes $|g_+|$; the blue dashed line, $|g_-|$; and the black line with dots (for the state that is initially unoccupied), $|(uv)_\pm|$. The initial states are, in (a) and (b), $|\Psi(0)\rangle = |\text{e.s.}\rangle = -|-(0)\rangle$ and, in (c) and (d), $|\Psi(0)\rangle = |\text{g.s.}\rangle = |+(0)\rangle$.The parameters are for (a) and (c) $\Gamma < 2\Omega_0$ with $\Gamma = 2\pi \times 0.159$ kHz, $\Omega_0 = 2\pi \times 79.578$ kHz, $b = 4 \times 10^{10}$ s^{-2}, and $t_f = 3$ ms and for (b) and (d) $\Gamma > 2\Omega_0$ with $\Gamma = 2\pi \times 799.775$ kHz, $\Omega_0 = 2\pi \times 79.578$ kHz, $b = 9 \times 10^{12}$ s^{-2}, and $t_f = 0.07$ ms.

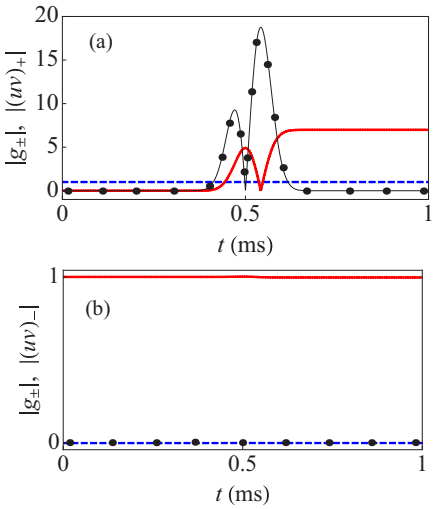

FIG. 7. (Color online) Plot of $|g_+|$ (red solid line), $|g_-|$ (blue dashed line), and $|(uv)_\pm|$ (black dots with or without a black line) for a CPR process when (a) $|\Psi(0)\rangle = |\text{g.s.}\rangle = |-(0)\rangle$ (least dissipative) and (b) $|\Psi(0)\rangle = |\text{e.s.}\rangle = |+(0)\rangle$ (most dissipative) for the parameters $\Gamma = 2\pi \times 3.183$ kHz, $\Omega_{\max} = 2\pi \times 0.159$ kHz, $a = 4 \times 10^8$ s^{-2}, $\Delta_0 = 2\pi \times 2$ Hz, and $t_f = 1$ ms.

In general though, $-(uv)_\pm(t)$ do not reproduce $g_\pm(t)$ accurately, even when the condition of first-order perturbation theory $g_m(t) \approx 1$ holds. A clear example taken from CPR is depicted in Fig. 7(a), where the remainder integral $\int_0^t v_+ du_+$ [see Eq. (23)] is not small, so $-(uv)_+(t)$ is quite different from $g_+(t)$ even though $g_-(t) \approx 1$ during the process. Contrast the failure of $-(uv)_+$ in Fig. 7(a) with the accurate fitting in Fig. 4(a). Integration by parts provides a formal series in powers of $\omega_{nm}(t)$, as shown in Appendix A, where the only critical points are the end points, but other points may play an important role. The approximation $g_n(t) \approx -(uv)_n(t)$, from the first term in Eq. (23), can also be found by assuming $u_n(t' < t) \approx u_n(t)$ in $g_n(t) = -\int_0^t u_n dv_n$ (we assume also that the contribution at $t = 0$ is negligible). This substitution, though, is not always permissible. Take, for example, $t = t_f$ in Figs. 4 and 7. Figure 8 demonstrates that the oscillation or otherwise of $e^{iW_{+-}}$ makes the u_+ contribution around $t_f/2$ either irrelevant (in Fig. 4) or quite significant (in Fig. 7). In the later case, the approximation based only on the critical point at t_f cannot be accurate. An alternative view making use of the complex-time plane to perform the integrals is provided in Appendix B. In general, accurate approximations of the $g_\pm(t)$ requires contour deformations in the complex time plane [23,35] to identify and take into account contributions from all relevant eigenvalue degeneracies and other critical points. In addition, crossings of Stokes lines [36] determine changes in the asymptotic behavior of the amplitudes [17]. While this type of analysis is possible for simple specific models and protocols [17,23,36], it may easily become intractable for moderately complex systems (such as a generic three-level system [23]) due to the proliferation of singularities [23]. An open question then is to bridge the gap between a simple condition such as (24) and more accurate conditions in generic cases.

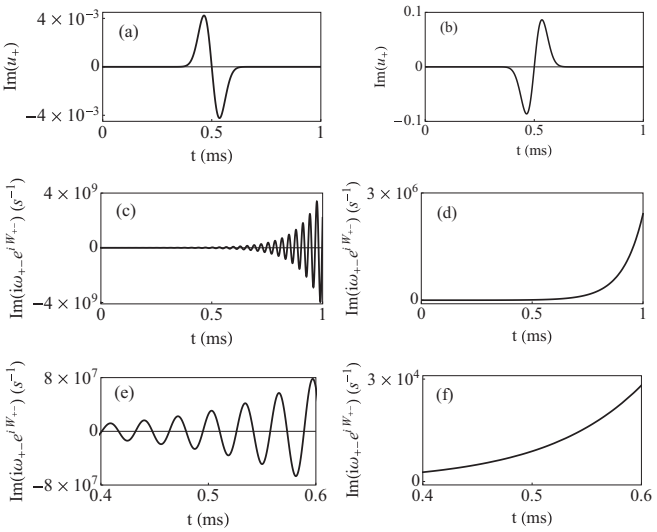

FIG. 8. Comparison of imaginary parts of integrand terms of g_+ [see Eqs. (21) and (22)] for the CPR process of Fig. 4(a), in (a), (c), and (e), and of Fig. 7(a), in (b), (d), and (f): (a) and (b) $\mathrm{Im}(u_+)$, (c) and (d) $\mathrm{Im}(i\omega_{+-}e^{iW_{+-}})$, and (e) and (f) zoom of (c) and (d) around the central time. The corresponding figures for the real parts are qualitatively similar.

VI. DISCUSSION

Adiabaticity is a key concept in quantum physics and its generalization to systems described by non-Hermitian dynamics requires the analysis of several possible formal extensions of the populations conserved for adiabatic dynamics in Hermitian systems. We have singled out among them the one that best identifies adiabatic following because it remains adiabatically invariant. Examples to illustrate its behavior have been drawn from CPR and LZ processes. A simple approximate expression has been also worked out by perturbation theory and partial integration, as well as higher orders in inverse powers of the transition frequency, for studying the adiabaticity of states different from the one initially occupied. It appears as a natural generalization of the usual condition for Hermitian systems. Its Hermitian counterpart is not infallible [37–40], so an accurate performance cannot be expected in general, as shown in the examples. This suggests many directions for future work: A systematic analysis and prediction of its possible failures is needed. In addition to the reasons found in its Hermitian counterpart, other elements have to be considered, such as the occurrence of NH degeneracies [17,27]. The simple approach to NH adiabaticity followed here, in exact or approximate forms, should also be contrasted with alternative views both conceptually and for specific applications. For example, in CPR, adiabaticity has been discussed in terms of the eigenstates of the Hermitian Hamiltonian without decay [with $\Gamma = 0$ in Eq. (27)] instead of the full Hamiltonian [31].

Further applications or extensions of this work may be in fields such as dissipative master equations [41,42], superadiabatic treatments [15,43,44], time-dependent dissipation rates [23], or non-Hermitian quantum adiabatic computation [45]. The formalism and concepts are also applicable beyond quantum physics, for example, to treat coupled waveguides [20].

ACKNOWLEDGMENTS

We are grateful to M. V. Berry for commenting on the original manuscript and to A. Peralta Conde and D. Sokolovski for discussions. We acknowledge funding by Grants No. IT472-10 and No. FIS2009-12773-C02-01 and the UPV/EHU Program No. UFI 11/55. S.I. acknowledges support from the Basque Government (Grant No. BFI09.39).

APPENDIX A: SECOND- AND THIRD-ORDER APPROXIMATIONS OF THE $g_n(t)$

Integrating the second term in Eq. (23) again by parts, as $\int_0^t v_n du_n = \int_0^t u_{1,n} dv_{1,n}$, where

$$u_{1,n} = \frac{\langle \hat{n}(t')|\dot{m}(t')\rangle + \langle \hat{n}(t')|\ddot{m}(t')\rangle}{[i\omega_{nm}(t')]^2} - \frac{\langle \hat{n}(t')|\dot{m}(t')\rangle i\dot{\omega}_{nm}(t')}{[i\omega_{nm}(t')]^3},$$

$$dv_{1,n} = i\omega_{nm}(t')e^{iW_{nm}(t')}dt',$$

we get

$$g_n(t) = \left\{ -\frac{\langle \hat{n}(t')|\dot{m}(t')\rangle}{i\omega_{nm}(t')} + \frac{\langle \dot{\hat{n}}(t')|\dot{m}(t')\rangle + \langle \hat{n}(t')|\ddot{m}(t')\rangle}{[i\omega_{nm}(t')]^2} - \frac{\langle \hat{n}(t')|\dot{m}(t')\rangle i\dot{\omega}_{nm}(t')}{[i\omega_{nm}(t')]^3} \right\} e^{iW_{nm}(t')}\Big|_0^t - \int_0^t v_{1,n} du_{1,n}.$$

We may integrate by parts the remainder integrals that appear at each step. First we rewrite $\int_0^t v_{1,n} du_{1,n} = \int_0^t u_{2,n} dv_{2,n}$, with

$$u_{2,n} = \frac{\langle \ddot{\hat{n}}(t')|\dot{m}(t')\rangle + 2\langle \dot{\hat{n}}(t')|\ddot{m}(t')\rangle + \langle \hat{n}(t')|\dddot{m}(t')\rangle}{[i\omega_{nm}(t')]^3} - \frac{[\langle \dot{\hat{n}}(t')|\dot{m}(t')\rangle + \langle \hat{n}(t')|\ddot{m}(t')\rangle]3i\dot{\omega}_{nm}(t')}{[i\omega_{nm}(t')]^4} - \frac{\langle \hat{n}(t')|\dot{m}(t')\rangle i\ddot{\omega}_{nm}(t')}{[i\omega_{nm}(t')]^4} - \frac{\langle \hat{n}(t')|\dot{m}(t')\rangle 3\dot{\omega}_{nm}^2(t')}{[i\omega_{nm}(t')]^5},$$

$$dv_{2,n} = i\omega_{nm}(t')e^{iW_{nm}(t')}dt'.$$

Thus,

$$g_n(t) = \left\{ -\frac{\langle \hat{n}(t')|\dot{m}(t')\rangle}{i\omega_{nm}(t')} + \frac{\langle \dot{\hat{n}}(t')|\dot{m}(t')\rangle + \langle \hat{n}(t')|\ddot{m}(t')\rangle}{[i\omega_{nm}(t')]^2} - \frac{\langle \hat{n}(t')|\dot{m}(t')\rangle i\dot{\omega}_{nm}(t') - \langle \ddot{\hat{n}}(t')|\dot{m}(t')\rangle}{[i\omega_{nm}(t')]^3} - \frac{2\langle \dot{\hat{n}}(t')|\ddot{m}(t')\rangle + \langle \hat{n}(t')|\dddot{m}(t')\rangle}{[i\omega_{nm}(t')]^3} + \frac{[\langle \dot{\hat{n}}(t')|\dot{m}(t')\rangle + \langle \hat{n}(t')|\ddot{m}(t')\rangle]3i\dot{\omega}_{nm}(t')}{[i\omega_{nm}(t')]^4} + \frac{\langle \hat{n}(t')|\dot{m}(t')\rangle i\ddot{\omega}_{nm}(t')}{[i\omega_{nm}(t')]^4} + \frac{\langle \hat{n}(t')|\dot{m}(t')\rangle 3\dot{\omega}_{nm}^2(t')}{[i\omega_{nm}(t')]^5} \right\} e^{iW_{nm}(t')}\Big|_0^t + \int_0^t v_{2,n} du_{2,n}.$$

Further integration by parts of the reminders generates a series with increasing powers of $\omega_{nm}(t)$ in the denominators. Similarly, the change $s = t/t_f$ and writing derivatives and integrals with respect to s provides a series in inverse powers of t_f.

APPENDIX B: COMPLEX TIME ANALYSIS

Figures 4(a) and 7(a) for CPR demonstrate that the approximation $g_+(t) \approx -(uv)_+(t)$ for the initially unoccupied state using integration by parts may be valid or it may fail. The approximation relies on the contribution to the integral near the boundary time t_f, so it fails when other critical points become important, as in Fig. 7(a). Consider the integral in Eq. (21) rewritten as $-\int h(t')e^{\Phi(t')}dt'$, with $h(t') = \langle \widehat{+}(t')|\partial_t|-(t')\rangle$ and $\Phi(t') = iW_{+-}(t')$. Figures 9(a) and 9(b) show the degeneracy points $E_+(t) = E_-(t)$ in the complex-time plane. They are branch cuts of the exponent Φ [see Figs. 9(c) and 9(d)] and in addition poles of the function h. The original integral goes along the real axis. The two cases studied correspond to two very different configurations of the function Φ in the complex-time plane, as shown in Figs. 9(e)–9(h). When the approximation works (see Fig. 4 and the left column in Fig. 9), Re(Φ) decreases towards the upper half plane so that a steepest-descent path from t_f, almost perpendicular to the real axis [see Fig. 9(e)], provides the dominant contribution to the integral. A path towards $t = 0$ can be drawn through the valley without giving any significant contribution to the integral [see Fig. 9(g)]. When the approximation fails [see Figs. 7, 9(b), 9(d), 9(f), and 9(h)], a steepest-descent path goes from t_f to $t = 0$ along the real axis [see Fig. 9(f)]. Upper and lower degenerate points are now at very similar heights [see Fig. 9(h)]. Here Re(Φ) decreases monotonically along the real line towards $t = 0$, but now the close singularities of the function h imply a strong disturbance and contribution around $t_f/2$.

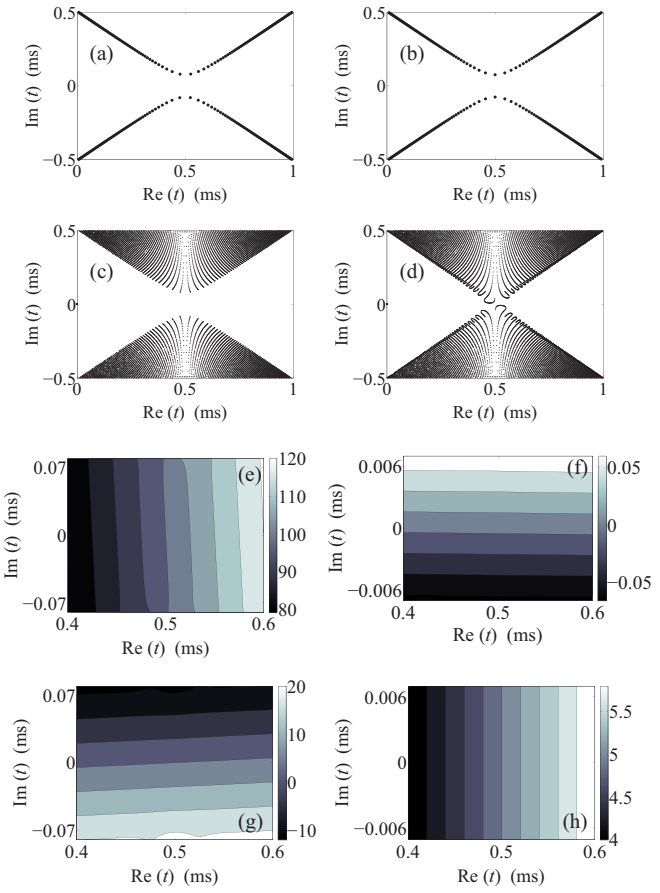

FIG. 9. (Color online) Complex time analysis of the integral for g_+ [see Eq. (21)] for the CPR process of Fig. 4(a), in (a), (c), (e), and (g), and of Fig. 7(a), in (b), (d), (f), and (h): (a) and (b) degeneracy points ($E_+ = E_-$), (c) and (d) branch cuts of the exponent Φ following the criterion in Fig. 3(a), (e) and (f) Im(Φ), and (g) and (h) Re(Φ). The contour maps show a rectangle around $t_f/2$ not including the singularities.

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