The role of the geometric phases in adiabatic population tracking for non-Hermitian Hamiltonians

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Abstract

The definition of instantaneous eigenstate populations for a dynamical non-self-adjoint system is not obvious. The naïve direct extension of the definition used for the self-adjoint case leads to inconsistencies; the resulting artifacts can induce a false inversion of population or a false adiabaticity. We show that the inconsistency can be avoided by introducing geometric phases in another possible definition of populations. An example is given which demonstrates both the anomalous effects and their removal by our approach.

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1. Introduction

The adiabatic approximation is currently a commonly used tool to study quantum dynamical systems [1]. Let $s = t/T$ be the reduced time (T being the total duration which is assumed to be very large). Let $|a, x(s)\rangle$ be an instantaneous eigenvector of a self-adjoint Hamiltonian $H(x(s))$ associated with a non-degenerate eigenvalue E_a, i.e.

$$H(x(s))|a, x(s)\rangle = E_a|a, x(s)\rangle. \tag{1}$$

Here H depends on the reduced time s from some classical parameters x. Starting from the initial state $\psi(0) = |a, x(0)\rangle$, the state vector propagation obeys the time-dependent Schrödinger equation

$$\frac{\mathrm{i}}{T}\frac{\partial \psi(sT)}{\partial s} = H(x(s))\psi(sT). \tag{2}$$

The adiabatic theorem [1, 2] states that the system continuously follows the same eigenstate $|a, x(s)\rangle$ if the Hamiltonian is gradually modified; that is,

$$\psi(sT) = c_a(s)|a, x(s)\rangle + \sum_{b \neq a} c_b(s)|b, x(s)\rangle \tag{3}$$

with

$$\forall b \neq a, \quad \left| \frac{c_b}{c_a} \right| \ll 1, \tag{4}$$

$|c_a(s)|^2$ being called the population of the state a, if the following adiabatic criterion is fulfilled:

$$\forall b \neq a, \quad |\langle b, x(s)| \frac{1}{T} \frac{d}{ds} |a, x(s)\rangle| = \left| \frac{\langle b, x(s)| \frac{1}{T} \frac{dH}{ds} |a, x(s)\rangle}{E_a(x(s)) - E_b(x(s))} \right|$$
$$\ll \min_{s \in [0,1]} |E_a(x(s)) - E_b(x(s))|, \tag{5}$$

which requires the satisfaction of the gap condition: $\exists g > 0, \forall s \quad |E_a(x(s)) - E_b(x(s))| > g$, and also slow time variations within the Hamiltonian $H(x(s))$. This leads to the wavefunction

$$\psi(sT) = \exp\left(-i\hbar^{-1} T \int_0^s E_a(x(s'))ds'\right) \exp\left(-\int_0^s A(x(s'))ds'\right) |a, x(s)\rangle + \mathcal{O}\left(\frac{1}{T}\right), \tag{6}$$

where

$$-i\hbar^{-1} T \int_0^s E_a(x(s)) \, ds$$

is the dynamic phase and

$$-\int_0^s A(x(s)) \, ds$$

is the geometric phase. The geometric phase generator is defined as

$$A(x) = \langle a, x|d|a, x\rangle \Rightarrow A(x(s)) \, ds = \langle a, x(s)| \frac{d}{ds} |a, x(s)\rangle ds. \tag{7}$$

Studies on adiabaticity and geometric phases can now be usefully extended to dissipative systems which use non-self-adjoint Hamiltonians to describe resonance phenomena [3–7]. When resonances are defined by some scattering boundary conditions, the resonance states are unbounded. This means that numerical and theoretical treatment of the resonances is a difficult task. Spectral deformation methods are commonly used to solve this problem. The first one, the complex scaling method [8], effectively transforms the resonance states into bound states. The Hamiltonian becomes non-self-adjoint, and the resonance calculations produce non-real eigenvalues and the associated eigenvectors. The real part of a resonance eigenvalue corresponds to the resonance energy and its imaginary part corresponds to the resonance width (the inverse of the resonance lifetime). The second approach is the optical potential method [9], which has similar properties. These two methods of resonance modeling involve non-self-adjoint Hamiltonians and are successfully used to treat molecular photodissociation problems [10–12]. This paper deals with non-Hermitian matrices. Such matrices can be viewed as effective Hamiltonians associated with the Hamiltonians of resonance problems. Effective Hamiltonian techniques use small Hamiltonians to describe complex systems without loss of information. The principal effective Hamiltonian techniques are the partitioning technique [13], the quantum KAM method [14], the adiabatic elimination method [14] and the Bloch wave operator method [13]. Small non-self-adjoint matrices have also been used as Hamiltonians to describe some photoionization phenomena modeled by bound states coupled with a structureless continuum (these states are then viewed as resonances) [15–17]. Finally, we should note that the formalism used in this paper could be used to treat open quantum systems [18–20] which are described by a Lindblad equation

$$i\hbar \frac{\partial \rho}{\partial t} = L(\rho),$$

where ρ is a density matrix (a traceless positive self-adjoint matrix) and the Lindbladian L is a 'superoperator' (here we deliberately show the i factor). For a finite-dimensional Hilbert space, $\dim \mathcal{H} = n$, the space of the density matrices can be identified with an n^2-dimensional Hilbert space $\mathcal{L}$ (usually called the Liouville space). In the Liouville space, the Lindblad equation takes the form of the usual Schrödinger equation. If the Lindbladian is reduced to be a commutator with a self-adjoint Hamiltonian, i.e. $L(\rho) = [H, \rho]$, then L is a self-adjoint operator in the Liouville space $\mathcal{L}$. Usually, the Lindbladian, however, is $L(\rho) = [H, \rho] - \frac{i}{2} \sum_k (\{\Gamma_k^\dagger \Gamma_k, \rho\} + 2\Gamma_k \rho \Gamma_k^\dagger)$, where the operators Γ_k model the different decohering processes ($\{.,.\}$ is the anticommutator). In this case, L is a non-self-adjoint operator in $\mathcal{L}$. The non-real eigenvalues of L (its resonances) are associated with the decoherence. This work can be applied to such a system, but for the sake of simplicity we will use only the name 'Hamiltonian', even though it could represent a Lindbladian in the Liouville space. For further explanations about the meaning of adiabatic approximation and geometric phases in an open quantum system, we refer the reader to [18, 19].

For non-self-adjoint Hamiltonians, the adiabatic theorem [21, 22] involves a criterion on the dissipation rate of the quantum system studied (i.e. on the imaginary part of the instantaneous eigenvalue considered). We should stress that in this paper we do not criticize these adiabatic theorems and we do not search for another adiabatic theorem. The problem we address is rather that of the interpretation of the adiabatic occupancy coefficients, from a pragmatic point of view, in order to obtain a better understanding of numerical results obtained with non-Hermitian Hamiltonians. Naively, we could imagine that the adiabatic approximation for dissipative quantum systems should take the form $\psi(sT) = \sum_b c_b(s)|b, x(s)\rangle$ with $\forall b \neq a$, $\left|\frac{c_b}{c_a}\right| \ll 1$. The following section shows that this approximation is inconsistent, since the populations $|c_b|^2$ are not well defined. Consequently, a better definition of the instantaneous populations is proposed in section 2. This definition is equivalent to the c-product condition (described in [3]) for the case of symmetric non-Hermitian Hamiltonians and remains valid even for the non-symmetric case. The illustrative example of a two-state dissipative system is then described in section 3, with an application to an adiabatic state flip [23, 24] which is generated by following a loop around an exceptional point in the parameter plane.

2. Populations of the instantaneous eigenvectors

For the sake of simplicity, we consider a non-self-adjoint Hamiltonian $H(x)$ of rank 2 (the discussion can easily be generalized to higher dimensions). We deal with a biorthogonal basis set and use the standard scalar product. Let $\{E_1(x), E_2(x)\}$ be the two instantaneous eigenvalues of $H(x)$ (assumed to be diagonalizable) and $\{|1, x\rangle, |2, x\rangle\}$ be the two associated eigenvectors, and let $\{|1*, x\rangle, |2*, x\rangle\}$ be the biorthogonal basis, that is,

$$H(x)|a, x\rangle = E_a(x)|a, x\rangle, \tag{8}$$

$$H(x)^\dagger |a*, x\rangle = \overline{E_a(x)}|a*, x\rangle, \tag{9}$$

$$\langle a*, x|b, x\rangle = \delta_{ab}. \tag{10}$$

(The bar denotes the complex conjugate.) We note that in certain highly symmetric cases (i.e. when $H^t = H$) $\{|a, x\rangle\}$ and $\{|a*, x\rangle\}$ are related by a simple complex conjugation rule (formalized by the c-product [25, 3]).

Let

$$A(x) = \begin{pmatrix} \langle 1*, x|d|1, x\rangle & \langle 1*, x|d|2, x\rangle \\ \langle 2*, x|d|1, x\rangle & \langle 2*, x|d|2, x\rangle \end{pmatrix} \tag{11}$$

be the matrix of the geometric phase generators and of the non-adiabatic coupling. Let

$$\psi(t) = U(t, 0)|1, x(s = 0)\rangle \tag{12}$$

be the wavefunction for an evolution $s \mapsto x(s)$ ($U(t, 0)$ being the evolution operator). As in conservative systems, we could write

$$\psi(sT) = c_1(s)|1, x(s)\rangle + c_2(s)|2, x(s)\rangle, \tag{13}$$

with $|c_1(s)|^2$ being the 'population' of the state 1 and $|c_2(s)|^2$ the 'population' of the state 2; the adiabatic approximation corresponds to the case where $|c_2|^2$ is negligible. However this definition presents a significant problem. In contrast to the conservative case, where we choose an orthonormal eigenbasis to represent the dynamics, the normalization convention is arbitrary for a biorthogonal basis. Indeed, if $(\{|1, x\rangle, |2, x\rangle\}, \{|1*, x\rangle, |2*, x\rangle\})$ constitutes a biorthogonal eigenvectors system, this is also the case for $\left(\{\widetilde{|1, x\rangle}, \widetilde{|2, x\rangle}\}, \{\widetilde{|1*, x\rangle}, \widetilde{|2*, x\rangle}\}\right)$ with

$$\widetilde{|a, x\rangle} = \lambda_a(x)|a, x\rangle \tag{14}$$

$$\widetilde{|a*, x\rangle} = (\overline{\lambda_a(x)})^{-1}|a*, x\rangle \tag{15}$$

for all arbitrary functions $\lambda_a(x) \in \mathbb{C}^*$. We must then set

$$\psi(sT) = \tilde{c}_1(s)\widetilde{|1, x(s)\rangle} + \tilde{c}_2(s)\widetilde{|2, x(s)\rangle} \tag{16}$$

with

$$\tilde{c}_a(s) = \frac{c_a(s)}{\lambda_a(x(s))}. \tag{17}$$

The population $|\tilde{c}_a|^2 = \frac{|c_a|^2}{|\lambda_a|^2}$ then depends on the arbitrary normalization convention. The calculation of the instantaneous populations then makes no sense, since the adiabatic multiplier c_1 can artificially grow if the normalization of $|a, x(s)\rangle$ decreases.

To solve this problem, we introduce a definition of the instantaneous populations using geometric phases. We set

$$\psi(sT) = d_1(s) \exp\left(-\int_0^s A_{11}(x(s'))\mathrm{d}s'\right)|1, x(s)\rangle + d_2(s) \exp\left(-\int_0^s A_{22}(x(s'))\mathrm{d}s'\right)|2, x(s)\rangle \tag{18}$$

with $\langle a, x(s = 0)|a, x(s = 0)\rangle = 1$. The instantaneous populations are now defined by $|d_a(s)|^2$. Immediately, we note that for the conservative case this definition coincides with the standard definition of the instantaneous populations since $|\mathrm{e}^{-\int_0^s A_{aa}(x(s'))\mathrm{d}s'}|^2 = 1$ in a self-adjoint system. (A_{aa} is purely imaginary; the standard definition of the instantaneous populations is invariant under arbitrary changes to the phase convention of the eigenvectors.) By making an arbitrary change in the normalization convention, we have

$$\tilde{A}_{aa}(x) = \widetilde{\langle a*, x|}\mathrm{d}\widetilde{|a, x\rangle} \tag{19}$$

$$= \frac{\mathrm{d}\lambda_a(x)}{\lambda_a(x)} + \langle a*, x|\mathrm{d}|a, x\rangle \tag{20}$$

$$= \mathrm{d}\ln\lambda_a(x) + A_{aa}(x). \tag{21}$$

We then have

$$\mathrm{e}^{-\int_0^s \tilde{A}_{aa}(x(s'))\mathrm{d}s'} = \frac{\lambda_a(x(0))}{\lambda_a(x(s))}\,\mathrm{e}^{-\int_0^s A_{aa}(x(s'))\mathrm{d}s'}. \tag{22}$$

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In order to preserve the initial condition, we set $\lambda_a(x(0)) = 1$. This leads to

$$\psi(sT) = d_1(s)\,\mathrm{e}^{-\int_0^s \tilde{A}_{11}(x(s'))\mathrm{d}s'}|\widetilde{1, x(s)}\rangle + d_2(s)\,\mathrm{e}^{-\int_0^s \tilde{A}_{22}(x(s'))\mathrm{d}s'}|\widetilde{2, x(s)}\rangle. \tag{23}$$

The definition of the instantaneous populations, $|d_a|^2$, is now invariant even in the event of arbitrary changes in the normalization convention. Here we insist on the fact that the coefficients d_a are more intrinsic than the coefficients c_a.

Owing to dissipation the total population strays away from 1 (except for $s = 0$). We have $1 - (|d_1|^2 + |d_2|^2) \geqslant 0$, but this is not a properly defined dissipation rate (i.e. $|d_1|^2 + |d_2|^2 \neq \|\psi\|^2$). The dissipation rate is given by $(1 - \|\psi(sT)\|^2)$ with

$$\|\psi(sT)\|^2 = \sum_{a,b} \overline{d_b(s)} d_a(s) \exp\left(-\int_0^s (A_{aa}(x(s')) + \overline{A_{bb}(x(s'))})\mathrm{d}s'\right) \times \langle b, x(s)|a, x(s)\rangle \tag{24}$$

$$= \sum_{a,b} \overline{d_b(s)}\eta_{ba}(s)d_a(s) \tag{25}$$

$$= D(s)^\dagger \eta(s)D(s) \tag{26}$$

with

$$D(s) = \begin{pmatrix} d_1(s) \\ d_2(s) \end{pmatrix}$$

and

$$\eta_{ab}(s) = \mathrm{e}^{-\int_0^s (A_{aa}(x(s')) + \overline{A_{bb}(x(s'))})\mathrm{d}s'}\langle b, x(s)|a, x(s)\rangle.$$

η constitutes an s-dependent scalar product for $D(s)$, the representation of the wave functions in the instantaneous (non-orthonormal) eigenbasis. We note that η is well defined since it is independent of the normalization convention, $\tilde{\eta} = \eta$. The scalar product matrix satisfies the following differential equation:

$$\frac{\mathrm{d}\eta}{\mathrm{d}s} = \hat{A}^\dagger \eta + \eta \hat{A} \tag{27}$$

with

$$\hat{A}_{ab}(s) = \langle a*, x(s)|\mathrm{e}^{\int_0^s A_{aa}(x(s'))\mathrm{d}s'}\frac{\mathrm{d}}{\mathrm{d}s}\left(\mathrm{e}^{-\int_0^s A_{bb}(x(s'))\mathrm{d}s'}|b, x(s)\rangle\right). \tag{28}$$

We can then write

$$\eta(s) = \left(\mathbb{T}\mathrm{e}^{\int_0^s \hat{A}(s')\mathrm{d}s'}\right)^\dagger \eta(0)\mathbb{T}\mathrm{e}^{\int_0^s \hat{A}(s')\mathrm{d}s'}, \tag{29}$$

where $\mathbb{T}\mathrm{e}$ is the s-ordered exponential (the Dyson series).

Finally, if we want the instantaneous total population to be consistent with the dissipation rate, then the instantaneous population must be defined as $\alpha(s)|d_a(s)|^2$ with $\alpha = \frac{D^\dagger \eta D}{D^\dagger D}$.

Using this analysis, we propose that the consistent adiabatic approximation is

$$\left|\frac{d_2}{d_1}\right| \ll 1 \tag{30}$$

and not $\left|\frac{c_2}{c_1}\right| \ll 1$. In a similar manner, the adiabatic criterion must be independent of the arbitrary normalization convention:

$$\mathrm{e}^{\int_0^s \mathfrak{Re}(A_{bb}(x(s')) - A_{aa}(x(s')))\mathrm{d}s'}\left|\langle b*, x(s)|\frac{1}{T}\frac{\mathrm{d}}{\mathrm{d}s}|a, x(s)\rangle\right|$$

$$= \mathrm{e}^{\int_0^s \mathfrak{Re}(A_{bb}(x(s')) - A_{aa}(x(s')))\mathrm{d}s'}\left|\frac{\langle b*, x(s)|\frac{1}{T}\frac{\mathrm{d}H}{\mathrm{d}s}|a, x(s)\rangle}{E_a(x(s)) - E_b(x(s))}\right|$$

$$\ll \min_{s\in[0,1]}|E_a(x(s)) - E_b(x(s))|. \tag{31}$$

The ratio $|d_2/d_1|$ indicates the magnitude of the deviation from an ideal adiabatic behavior following the state $|1, x(s)\rangle$. The limit case when T tends to infinity corresponds to the adiabatic theorems [21, 22].

From the adiabatic approximation, one can wish to project the adiabatic states onto the initial diabatic basis $|a, x(s = 0)\rangle$. Evidently, assuming for example that one adiabatic state $|a, x(s)\rangle$ is effectively followed by the wavefunction, it is important not to project it directly onto the diabatic basis to obtain the dynamics in terms of diabatic populations but rather to take into account the geometric and dynamic factors: for example, if the diabatic basis is orthonormal and we assume a dynamics which follows the adiabatic state no 1, then the population of the first diabatic state is $|\langle 1, x(0)|1, x(s)\rangle|^2 \exp\left\{-2\int_0^s \Re\left[A_{11}(x(s'))\right] ds'\right\}$ or equivalently $|\langle 1, x(0)|\widehat{1, x(s)}\rangle|^2 \exp\left\{-2\int_0^s \Re\left[\tilde{A}_{11}(x(s'))\right] ds'\right\}$ [see (18) and (23)].

We should point out that the use of the parallel transport condition, i.e. the definition of the populations with eigenvectors $\{|\widehat{a, x(s)}\rangle\}_a$ and $\{|\widehat{a*, x(s)}\rangle\}_a$, such that

$$\langle\widehat{a*, x(s)}|\frac{d}{ds}|\widehat{a, x(s)}\rangle = 0 \tag{32}$$

implicitly takes into account the instantaneous population definition which includes the geometric phases. Indeed, it is easy to show that $\{|\widehat{a, x(s)}\rangle\}_a$ are related to an arbitrary set of eigenvectors $\{|a, x\rangle\}_a$ by

$$|\widehat{a, x(s)}\rangle = e^{-\int_0^s A_{aa}(x(s'))ds'}|a, x(s)\rangle. \tag{33}$$

In the particular case of a symmetric matrix, the left eigenvectors are the complex conjugates of the right eigenvectors, so that the parallel transport condition is also equivalent to the c-product normalization condition for the eigenvectors $|a, x(s)_{\text{c.p.}}\rangle$, fixed by [3]

$$\overline{\langle a, x(s)_{\text{c.p.}}|}a, x(s)_{\text{c.p.}}\rangle = 1. \tag{34}$$

The result of this paper could be expressed without explicit reference to the geometric phases by saying that the treatment of the population tracking for non-Hermitian systems necessary needs to impose the parallel transport condition (whereas this is not necessary for Hermitian systems). Nevertheless, we prefer here to make the geometric phases appear explicitly. Indeed, the $\{|\widehat{a, x(s)}\rangle\}_a$ are defined only along the path in the parameter space defined by $s \mapsto x(s)$; for a different path $s \mapsto x'(s)$ the eigenvectors $\{|\widehat{a, x(s)}\rangle'\}_a$ are different. It is then more general to consider $\{|a, x\rangle\}_a$ (without a parallel transport condition) which are defined globally on the whole of the parameter space.

Moreover, we note that we cannot use the parallel transport condition to define the eigenvectors if the path is closed $x(s = 0) = x(s = 1)$ because of the double definition of the eigenvectors at $x(0) = x(1)$:

$$|\widehat{a, x(1)}\rangle = e^{-\int_0^1 A_{aa}(x(s))ds}|a, x(1)\rangle \neq |a, x(0)\rangle = |\widehat{a, x(0)}\rangle. \tag{35}$$

The impossibility of giving a single definition of the eigenvectors in the parallel transport condition $e^{-\int_0^1 A_{aa}(x(s))ds}$ is called the holonomy of the parallel transport.

The following section illustrates that numerical artifacts due to bad definitions of the populations can induce a false adiabaticity or a false inversion of population in numerical simulations.

3. Illustrative example

Definition (18) is relevant for non-Hermitian symmetric or non-symmetric matrices. While the formalism used here should work for larger, more realistic Hamiltonians and for

Floquet-type Hamiltonians, we study here a low-dimensional illustrative example for which the data can be shown conveniently. Let the parameter-dependent Hamiltonian be

$$H(w, z) = \begin{pmatrix} 0 & w \\ \bar{w} & 2z \end{pmatrix} = \begin{pmatrix} 0 & \Omega e^{i\phi} \\ \Omega e^{-i\phi} & 2\Delta - i\frac{\Gamma}{2} \end{pmatrix} \tag{36}$$

$(w, z) \in \mathbb{C}^2$. This Hamiltonian is associated with a quantum bound state coupled to a quantum resonance (with resonance width Γ) by a laser field with amplitude Ω and phase ϕ. The laser field is quasi-resonant with the transition from the bound state to the resonance with a detuning value equal to Δ. We assume that we can modulate the complex numbers (w, z) to generate a dynamics.

3.1. False adiabaticity

The spectrum of H is

$$E_1(w, z) = z - \sqrt{|w|^2 + z^2} = z - v \tag{37}$$

$$E_2(w, z) = z + \sqrt{|w|^2 + z^2} = z + v, \tag{38}$$

where $v = \sqrt{|w|^2 + z^2} = z\sqrt{1 + \frac{|w|^2}{z^2}}$. (We choose the Riemann sheet such that $\sqrt{z^2} = z$.) We restrict our attention to the parameters (w, z) such that $\Im m(E_2 - E_1) = 2\Im m(v) < 0$ (E_1 is the less dissipative).

We can easily verify that the eigenvectors of $H(w, z)$ are

$$|1, w, z\rangle = \gamma_1 \begin{pmatrix} z + v \\ -\bar{w} \end{pmatrix} \tag{39}$$

$$|2, w, z\rangle = \gamma_2 \begin{pmatrix} z - v \\ -\bar{w} \end{pmatrix}, \tag{40}$$

where γ_a are the appropriate factors to fix the initial norm of the basis vectors to 1, i.e.

$$\gamma_1 = \frac{1}{\sqrt{(|z(0) + v(0)|^2 + |w(0)|^2)}} \tag{41}$$

$$\gamma_2 = \frac{1}{\sqrt{(|z(0) - v(0)|^2 + |w(0)|^2)}}. \tag{42}$$

The biorthogonal basis set is

$$|1*, w, z\rangle = \frac{1}{2\bar{v}(\bar{v} + \bar{z})\gamma_1^2} |1, w, \bar{z}\rangle \tag{43}$$

$$|2*, w, z\rangle = \frac{1}{2\bar{v}(\bar{v} - \bar{z})\gamma_2^2} |2, w, \bar{z}\rangle. \tag{44}$$

The associated geometric phase generators are

$$A_{11} = \frac{\bar{w}\dot{w} + w\dot{\bar{w}}}{4v^2} + \frac{w\dot{\bar{w}}}{2v(v + z)} + \frac{(z + v)\dot{z}}{2v^2} \tag{45}$$

$$A_{22} = \frac{\bar{w}\dot{w} + w\dot{\bar{w}}}{4v^2} + \frac{w\dot{\bar{w}}}{2v(v - z)} - \frac{(v - z)\dot{z}}{2v^2}. \tag{46}$$

We can verify that another possible eigenstate 1 reads

$$\widetilde{|1, w, z\rangle} = \frac{\gamma_1}{\beta} \begin{pmatrix} w \\ z - v \end{pmatrix} \tag{47}$$

with

$$|1, w, z\rangle = \beta \frac{v + z}{w} \widetilde{|1, w, z\rangle} \tag{48}$$

and

$$\beta = \frac{w(0)}{v(0) + z(0)}. \tag{49}$$

The factor β ensures that $|1, w(0), z(0)\rangle = \widetilde{|1, w(0), z(0)\rangle}$ in order to preserve the initial condition. We assume that $\beta \neq 0$. The associated biorthogonal eigenvector is

$$\widetilde{|1*, w, z\rangle} = \frac{|\beta|^2}{2\bar{v}(\bar{v} - \bar{z})\gamma_1^2} \widetilde{|1, w, \bar{z}\rangle}. \tag{50}$$

The normalization factor between the two conventions approaches zero at the limit $|w| \to 0$,

$$\lim_{|w| \to 0} \beta \frac{w}{v + z} = 0. \tag{51}$$

With this normalization, the first geometric phase generator becomes

$$\tilde{A}_{11} = \frac{\bar{w}\dot{w} + w\dot{\bar{w}}}{4v^2} + \frac{\bar{w}\dot{w}}{2v(v - z)} - \frac{(v - z)\dot{z}}{2v^2}. \tag{52}$$

These properties induce the following analysis. Let

$$\psi(sT) = d_1(s) \, \mathrm{e}^{-\int_0^s \tilde{A}_{11}(s')\mathrm{d}s'} |1, \widetilde{w(s), z(s)}\rangle + d_2(s) \, \mathrm{e}^{-\int_0^s A_{22}(s')\mathrm{d}s'} |2, w(s), z(s)\rangle \tag{53}$$

be the solution to the Schrödinger equation for the evolution $s \mapsto (w(s), z(s))$ with the initial state $\psi(0) = |1, w(0), z(0)\rangle$. We suppose that the adiabatic approximation is valid, i.e. $\left| \frac{d_2}{d_1} \right| \ll 1$. If we consider the naive definition of the population by setting

$$\psi(sT) = c_1(s)|1, w(s), z(s)\rangle + c_2(s)|2, w(s), z(s)\rangle,$$

then the quotient

$$\left| \frac{c_1}{c_2} \right| = \frac{1}{\beta} \frac{|w|}{|z + v|} \left| \frac{\tilde{c}_1}{c_2} \right| \tag{54}$$

$$= \frac{1}{\beta} \frac{|w|}{|z + v|} \left| \frac{d_1}{d_2} \right| \mathrm{e}^{\int_0^s \Re\mathrm{e}(A_{22}(s') - \tilde{A}_{11}(s'))\mathrm{d}s'} \tag{55}$$

with $\psi(sT) = \tilde{c}_1(s)|1, \widetilde{w(s), z(s)}\rangle + c_2(s)|2, w(s), z(s)\rangle$. We note that if $\Im\mathrm{m}(w) = 0$, then $\Re\mathrm{e}(A_{22} - \tilde{A}_{11}) = 0$ and $\left| \frac{c_1}{c_2} \right| = \frac{|w|}{|\beta||z+v|} \left| \frac{d_1}{d_2} \right|$. The limit (51) can induce

$$|w| \ll 1 \Rightarrow \left| \frac{d_2}{d_1} \right| \ll 1 \text{ and } \left| \frac{c_1}{c_2} \right| \ll 1. \tag{56}$$

Thus we observe a false non-adiabaticity due to the badly defined populations. In this case, we also have a false population inversion (in the sense that population 1 is negligible with respect to population 2 using the badly defined populations, while the well-defined populations give the inverse result).

Conversely, let $\psi(sT)$ (cf (53)) be the solution to the Schrödinger equation for an evolution starting with an initial state $\psi(0) = |2, w(0), z(0)\rangle$ such that the adiabatic approximation is
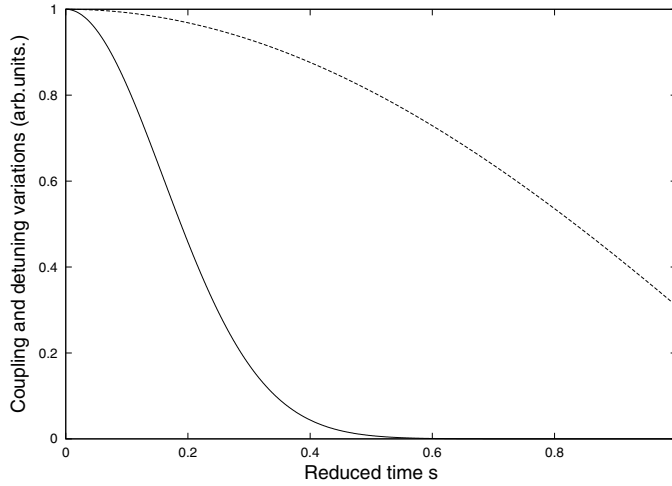
Figure 1. Time variations of the Rabi frequency w (line) and of the detuning $\Re e(z)$ (dashes).

not satisfied, i.e. for s sufficiently large, $|d_1| \sim |d_2|$. By the same arguments, if $|w| \ll 1$, then we have

$$\left| \frac{d_1}{d_2} \right| \sim 1 \quad \text{and} \quad \left| \frac{c_1}{c_2} \right| \ll 1. \tag{57}$$

In this case, we obtain a false adiabaticity due to the badly defined populations.

Figure 1 shows a simple example of a Gaussian variation for $w(s)$ (coupling) and a decreasing cosine function for $\Re e(z)$ (detuning), so that $|w(t)| \simeq 0$ near the end of the considered time interval [0, 100]. The chosen functions are

$$w(s) = w_0 \, e^{-\frac{s^2}{2\sigma^2}} \tag{58}$$

$$\Delta(s) = \Re e(z(s)) = \Delta_0 \cos(0.4\pi s) \tag{59}$$

with $w_0 = 1$, $\Delta_0 = 0.5$, $\Gamma = 0.1$ or 0.2 and $\sigma = 0.16$. This elementary example perfectly illustrates our assertions. Figure 2 corresponds to the case of a false inversion of population, beginning with the state $|1, w(0), z(0)\rangle$. $|\frac{c_2}{c_1}|$ becomes very large when $s > 0.8$, although $|\frac{d_2}{d_1}|$ remains very small for the duration of the interaction (using the definition which takes the geometric phases into account to compensate for the unstable norm of the basis vectors). This is consistent with our analysis because this false inversion of populations occurs when $w(s)$ becomes very small due to the Gaussian function. Moreover, we note the uncontrolled increase in c_1 and c_2, both reaching values larger than 1.

Figure 3 shows the principal cause of this problem (the uncontrollable variations in the norms of $|1, w, z\rangle$ and $|2, w, z\rangle$) and also the exact compensation obtained with the exponential of the geometric phases, leading to two stable unitary norms (since we have taken the precaution of setting the initial norms to 1).

In contrast, figure 4 illustrates the inverse phenomenon of false adiabaticity. The initial state is $|2, w(0), z(0)\rangle$. Thus, the ratio $|\frac{c_1}{c_2}|$ stays under the value of 0.01 as if it were an adiabatic evolution, while $|\frac{d_1}{d_2}|$ increases, with two components of the same order of magnitude ($d_1 \simeq d_2$) at the end of the interval.
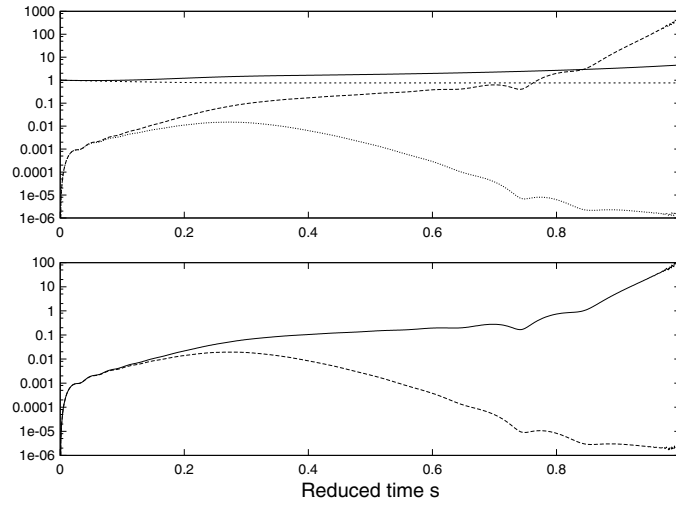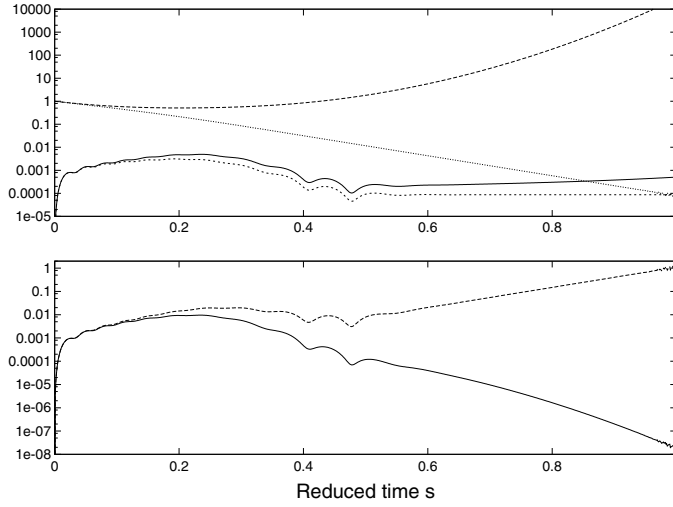
Figure 2. Top: $|c_1(s)|$ (line), $|c_2(s)|$ (long dashes), $|d_1(s)|$ (short dashes), $|d_2(s)|$ (dots); bottom: ratios $|c_2(s)/c_1(s)|$ (line) and $|d_2(s)/d_1(s)|$ (dashes). The initial state is $|1, w(0), z(0)\rangle$. $\Gamma = 0.1$. A logarithmic scale is used for the *y*-axis.
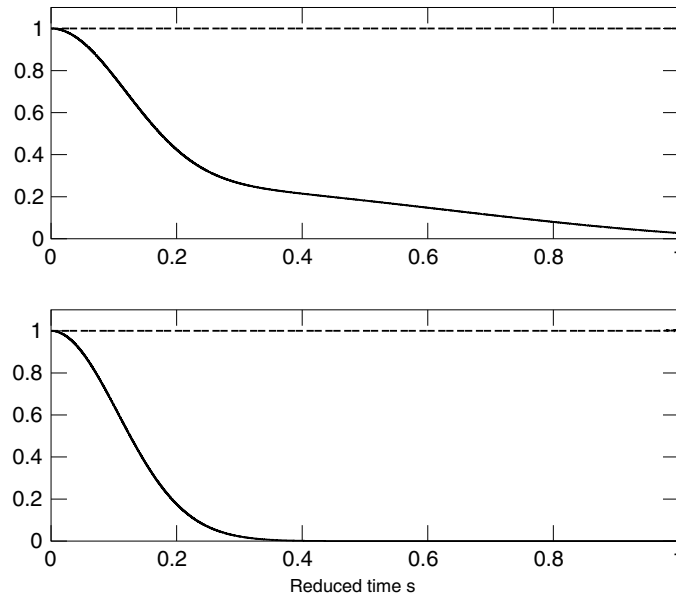
Figure 3. Top: $\langle 1, w, z|1, w, z\rangle$ (line), $\langle 1, w, z|1, w, z\rangle \times |e^{\int_0^s A_{11}(s')ds'}|^2$ (dashed line). Bottom: $\langle 2, w, z|2, w, z\rangle$ (line), $\langle 2, w, z|2, w, z\rangle \times |e^{\int_0^s A_{22}(s')ds'}|^2$ (dashed line). This corresponds to the case of a false inversion of population with $\Gamma = 0.1$.

3.2. Closed loop around an exceptional point in the parameter space

If Γ and ϕ are fixed, then the matrix of (36) has two exceptional points in the parameter plane (Ω, Δ). They are located at $(\Omega, \Delta) = (\pm\Gamma/4, 0)$. At these points, the two eigenvalues

Figure 4. Top: $|c_1(s)|$ (line), $|c_2(s)|$ (long dashes), $|d_1(s)|$ (short dashes), $|d_2(s)|$ (dots); bottom: ratios $|c_1(s)/c_2(s)|$ (line) and $|d_1(s)/d_2(s)|$ (dashes). The initial state was $|2, w(0), z(0)\rangle$. $\Gamma = 0.2$. A logarithmic scale is used for the *y*-axis.

and the two eigenvectors coalesce. If a closed loop that encircles a single exceptional point is followed in the parameter space, then the adiabatic basis is transported so as to have the following property [4]:

$$
\begin{aligned}
|1(s = 1)\rangle &= \nu_1|2(s = 0)\rangle \\
|2(s = 1)\rangle &= \nu_2|1(s = 0)\rangle,
\end{aligned}
\tag{60}
$$

where ν_1 and ν_2 are two complex numbers. If the dynamics is adiabatic, starting with one of the eigenstates, $|1(s = 0)\rangle$ leads to a final state $|1(s = 1)\rangle$ which is proportional to $|2(s = 0)\rangle$. This interchange is called an adiabatic flip. This interesting form of degeneracy in non-Hermitian quantum problems is the subject of several recent papers, involving both theoretical [23, 24, 26–28] and experimental [29, 30] studies. References [23, 26] deal with a symmetric matrix and show that beginning the loop with one state is favorable to an adiabatic behavior which leads to an adiabatic flip (interchange), while beginning with the other one (the more dissipative one) induces strong non-adiabatic couplings and state exchange during the process, whatever the time duration. The occupancy coefficients of the two states and the states themselves are exchanged during the loop, leading finally to the absence of flip. This is consistent with the conditions associated with the applicability of the adiabatic theorem [21, 22]. We can now confirm these results by our calculations and also extend them to the non-symmetric case by using definition (18).

3.2.1. Symmetric case.   We choose the parameters

$$
\begin{aligned}
&T = 100, \\
&z(s) = \Delta - i\Gamma/4 \\
&\text{with } \Gamma = 0.5 \text{ and } \Delta(s) = 0.24\,\Gamma \sin(2\pi s), \\
&w(s) = \Omega(s) = \frac{\Gamma}{4} + 0.24\,\Gamma \cos(2\pi s).
\end{aligned}
\tag{61}
$$
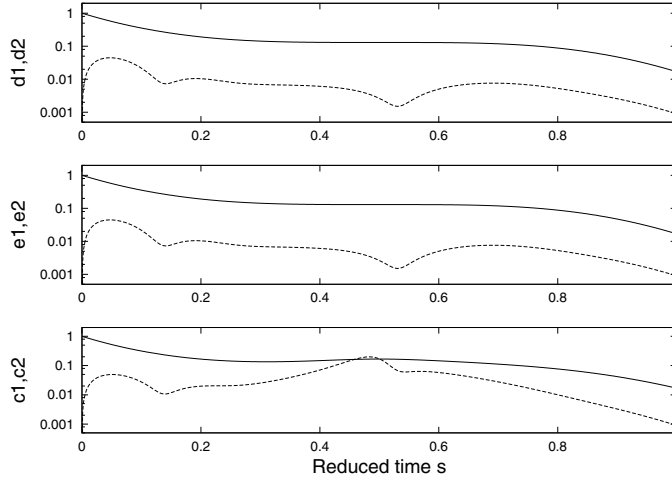
Figure 5. Top: $|d_1(s)|$ (line), $|d_2(s)|$ (dashes); middle: $|e_1(s)|$ (line), $|e_2(s)|$ (dashes); bottom: $|c_1(s)|$ (line), $|c_2(s)|$ (dashes). The initial state is $|1, w(0), z(0)\rangle$. A logarithmic scale is used for the *y*-axis.

We calculate the different adiabatic multipliers $c_1(s)$, $c_2(s)$ and $d_1(s)$, $d_2(s)$ following the adiabatic eigenstates by using the two conventions defined above. We also calculate results using a third convention which corresponds to the c-product normalization (34) and which gives the coefficients

$$e_1 = \overline{\langle 1, w(s), z(s)_{\text{c.p.}}|}\psi(sT)\rangle, \tag{62}$$

$$e_2 = \overline{\langle 1, w(s), z(s)_{\text{c.p.}}|}\psi(sT)\rangle \tag{63}$$

such that

$$|\psi(sT)\rangle = e_1(s)|1, w(s), z(s)_{\text{c.p.}}\rangle + e_2(s)|2, w(s), z(s)_{\text{c.p.}}\rangle. \tag{64}$$

This c-product normalization is adjusted so as to begin with the same initial condition $(e_1, e_2) = (1, 0)$ (or $(e_1, e_2) = (0, 1)$) as the two others. Figures 5 and 6 correspond to the dynamics issuing from the initial states $|1, w(0), z(0)\rangle$ and $|2, w(0), z(0)\rangle$, respectively. The $|c_1|$ and $|c_2|$ curves seem to indicate a non-adiabatic behavior, but are not numerically significant. The evolution of e_1 and e_2 is exactly the same as the evolution of d_1 and d_2. We see an adiabatic evolution in figure 5 for the dynamics issuing from $|1, w(0), z(0)\rangle$. The final state $|1, w(1), z(1)\rangle$ is predominantly occupied at the end of the loop, but owing to the flip of the eigenstates we do have an adiabatic flip. When the initial state is $|2, w(0), z(0)\rangle$ (figure 6), the non-adiabatic exchange of populations during the first part of the loop induces a final state near to state $|1, w(1), z(1)\rangle \propto |2, w(0), z(0)\rangle$ and there is no flip.

3.2.2. Non-symmetric case. The adiabatic loop is the same, but the only difference from the previous case is that the off-diagonal elements are now complex conjugates, so that the left eigenvectors are not the complex conjugate of the right eigenvectors. We set

$$w(s) = \Omega(s)\, e^{i\phi} = \left(\frac{\Gamma}{4} + 0.24\, \Gamma \cos(2\pi s)\right) e^{i\frac{\pi}{4}} \tag{65}$$
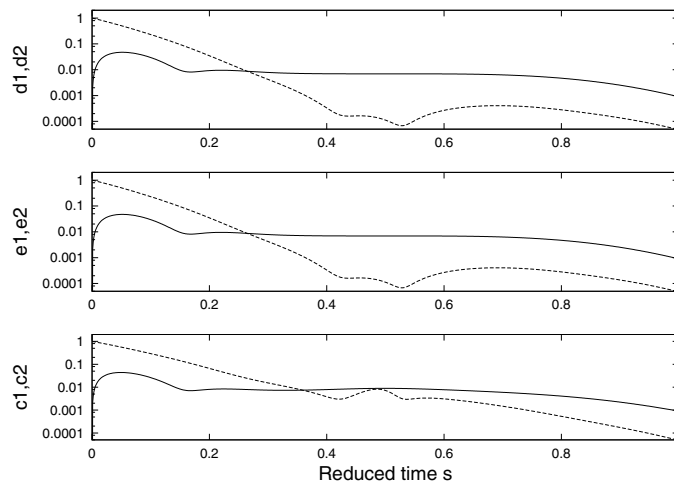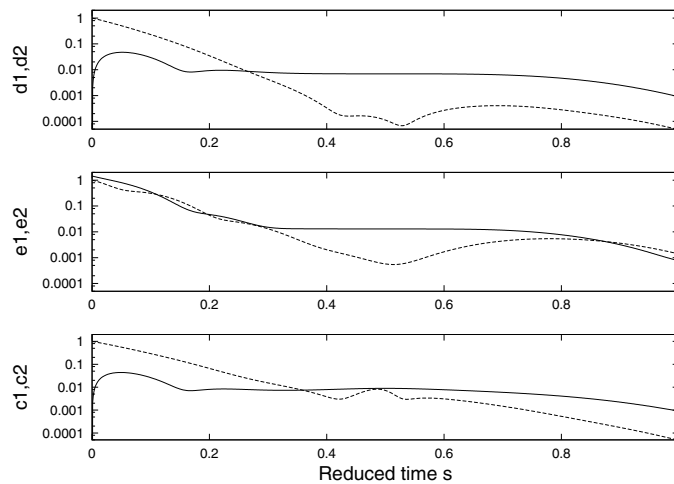
Figure 6. Same as figure 5 with the initial state $|2, w(0), z(0)\rangle$.
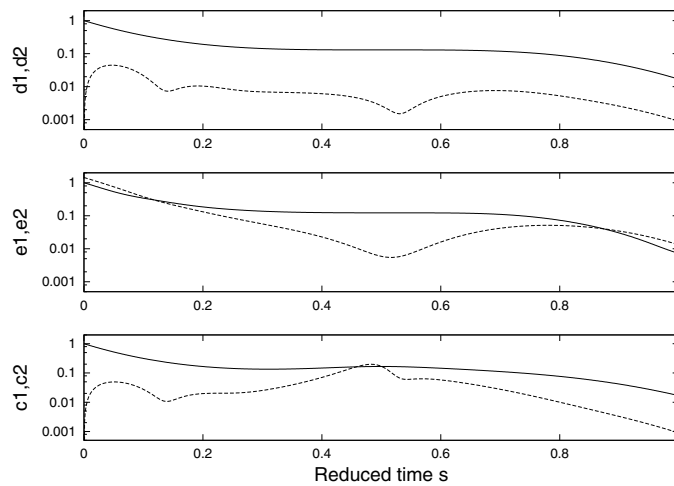
Figure 7. Top: $|d_1(s)|$ (line), $|d_2(s)|$ (dashes); middle: $|e_1(s)|$ (line), $|e_2(s)|$ (dashes); bottom: $|c_1(s)|$ (line), $|c_2(s)|$ (dashes). The initial state is $|1, w(0), z(0)\rangle$. A logarithmic scale is used for the y-axis.

Figures 7 and 8 show the evolution of the occupancy coefficients with the different definitions, beginning respectively with the initial state $|1, w(0), z(0)\rangle$ and $|2, w(0), z(0)\rangle$. We clearly see that it is no longer possible to use a c-product-type normalization: (63) should not be used in this case. The coefficients c_1 and c_2 continue not to be numerically significant. Only the coefficients d_1 and d_2 can be used in the present case and they show the same behavior as for the symmetric case.

Figure 8. Same as figure 7 with the initial state $|2, w(0), z(0)\rangle$.

4. Conclusion

This paper should be regarded as a simple clarification about the difficult interpretation of calculations on dissipative quantum systems described by non-Hermitian Hamiltonians and about the use of state populations as important observables, especially for studies on adiabatic phenomena. When one works with dissipative quantum systems, the erratic time evolution of the norm of the adiabatic eigenvectors can create difficulties in answering the question: what is the relevant definition of a population? When the eigenvectors are calculated numerically (for large matrices), there is no reason for them to be continuously transformed from one point to another in time; thus, the norm variations can appear to be quite disordered (worse than in our semi-analytic example).

Seemingly, the easiest intuitive solution is to artificially normalize the 'right' eigenvectors as if we were working with an orthogonal basis set, but this is not a coherent way to work. We have shown that it is much preferable to compensate for the erratic variations in the norm of the adiabatic basis set by including the exponentials of the geometric phases in the basis vector decomposition, leading to an invariant definition of the populations under arbitrary changes of the normalization choice.

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