Improving shortcuts to adiabaticity by iterative interaction pictures

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Different techniques to speed up quantum adiabatic processes are currently being explored for applications in atomic, molecular, and optical physics, such as transport, cooling and expansion, wave-packet splitting, or internal state control. Here we examine the limitations and capabilities of superadiabatic iterations to produce a sequence of shortcuts to adiabaticity. The general formalism is worked out as well as examples for population inversion in a two-level system.

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I. INTRODUCTION

There is currently much interest in speeding up quantum adiabatic processes in fields such as fast cold-atom or ion transport, expansions, wave-packet splitting, or internal state population and state control [1]. Accelerating adiabatic protocols is also of interest beyond the quantum domain, for example to engineer robust mode converters of reduced length in optical waveguides [2,3]. For many of these applications, several formal solutions to finding a shortcut to adiabatic dynamics are known, but the resulting operation may in practice be too costly energetically, or difficult to implement because of the structure or the values of the driving Hamiltonian matrix elements. This motivates the search for shortcut-generating methods that improve the applicability of the speeding-up protocols iteratively or otherwise [4]. Iterative methods in which the energy of the system or the external resources needed decrease with each iteration, at least up to some critical iteration, are particularly appealing in this regard. The main aim of this paper is precisely to develop further and explore the limits and capabilities of an iterative scheme that produces sequences of shortcut-driving Hamiltonians, based on nested, "superadiabatic" interaction pictures [5–10].

To understand the method, we shall now delve into a more detailed description of the concepts involved and the immediate precedents. Demirplack and Rice [5–7] and Berry [9] proposed the addition of a suitable "counterdiabatic" term $H_{\rm cd}^{(0)}(t)$ to the time-dependent Hamiltonian $H_0(t)$, such that the system follows exactly the adiabatic dynamics of $H_0(t)$. The counterdiabatic term suppresses transitions in the instantaneous eigenbasis $\{|n_0(t)\rangle\}$ of $H_0(t)$, $H_0(t)|n_0(t)\rangle = E_n^{(0)}(t)|n_0(t)\rangle$, but allows for transitions in the instantaneous eigenbasis of the full Hamiltonian $H_0 + H_{\rm cd}^{(0)}$. Experiments that implement these ideas have been recently performed in different two-level systems [11,12]. The same $H_{\rm cd}^{(0)}(t)$ also appears naturally when studying the adiabatic approximation of the reference system, the one that evolves with $H_0(t)$; see, e.g., [13]. The reference system behaves adiabatically, following the eigenstates of $H_0(t)$, when the counterdiabatic term is negligible, and the adiabatic approximation is close to the actual dynamics. This is made evident in an interaction picture (IP) based on the unitary transformation $A_0(t) = \sum_n |n_0(t)\rangle\langle n_0(0)|$. [The "parallel-transport" condition $\langle n_0(t)|\dot{n}_0(t)\rangle = 0$ is assumed hereafter to define the phases.] From the Schrödinger equation $i\hbar\partial_t|\psi_0(t)\rangle = H_0(t)|\psi_0(t)\rangle$ and defining $|\psi_1(t)\rangle = A_0^\dagger|\psi_0(t)\rangle$, the IP equation $i\hbar\partial_t|\psi_1(t)\rangle = H_1(t)|\psi_1(t)\rangle$ is deduced, where $H_1(t) = A_0^\dagger(t)[H_0(t) - K_0(t)]A_0(t)$ is the effective IP Hamiltonian and $K_0(t) = i\hbar\dot{A}_0(t)A_0^\dagger(t)$ is a coupling term. If $K_0(t)$ is zero or negligible, $H_1(t)$ becomes diagonal in the basis $\{|n_0(0)\rangle\}$, so that the IP equation becomes an uncoupled system with solutions

$$|\psi_1(t)\rangle = U_1(t)|\psi_1(0)\rangle, \tag{1}$$

where

$$U_1(t) = \sum_n |n_0(0)\rangle e^{-\frac{i}{\hbar}\int_0^t E_n^{(0)}(t')dt'}\langle n_0(0)| \tag{2}$$

is the unitary evolution operator for the uncoupled system. Correspondingly, from $|\psi_0(t)\rangle = A_0(t)|\psi_1(t)\rangle$,

$$\left|\psi_0^{(1)}(t)\right\rangle = \sum_n |n_0(t)\rangle e^{-\frac{i}{\hbar}\int_0^t E_n^{(0)}(t')dt'}\langle n_0(0)|\psi_0(0)\rangle, \tag{3}$$

where we have used $|\psi_1(0)\rangle = |\psi_0(0)\rangle$ since $A_1(0) = 1$ by construction. The same solution, which, for a nonzero $K_0(t)$, is only approximate, may become exact by adding to the IP Hamiltonian the counterdiabatic term $A_0^\dagger(t)K_0(t)A_0(t)$. This requires an external intervention and changes the physics of the original system, so that $U_1(t)$ describes the evolution exactly. In the IP, the modified Hamiltonian is $H^{(1)}(t) = H_1(t) + A_0^\dagger(t)K_0(t)A_0(t) = A_0^\dagger(t)H_0(t)A_0(t)$, and in the Schrödinger picture (SP) the additional term becomes simply K_0. The modified Schrödinger Hamiltonian is $H_0^{(1)}(t) = H_0(t) + K_0(t)$, so we identify $H_{\rm cd}^{(0)}(t) = K_0(t)$. A "small" coupling term $K_0(t)$ that makes the adiabatic approximation a good one also implies a small counterdiabatic manipulation, but, irrespective of the size of $K_0(t)$, $H_0^{(1)}(t)$ provides a shortcut to slow adiabatic following because it keeps the populations in the instantaneous basis of $H_0(t)$ invariant, in particular at the final time t_f. Moreover, if $K_0(0) = 0$ and $K_0(t_f) = 0$, then $H_0^{(1)} = H_0$ at $t = 0$ and $t = t_f$. This is useful in practice to ensure the continuity of the Hamiltonian at the boundary times: usually $H_0(t < 0) = H_0(0)$ and $H_0(t > t_f) = H_0(t_f)$, so $K_0(t < 0) = K_0(t > t_f) = 0$, i.e., $H_0(t)$ is the actual Hamiltonian before and after the process.

The previous formal framework may be repeated iteratively to define IPs further by diagonalizing the effective Hamiltonians of each IP. These iterations were used to establish *generalized adiabatic invariants* and *adiabatic invariants of nth order* by Garrido [10]. Berry also used this iterative

procedure to calculate a sequence of corrections to Berry's phase for cyclic processes with finite slowness, and introduced the concept of "superadiabaticity" [8]. For later developments and applications, see, e.g., [4,7,11,14–21].

Superadiabatic iterations are best understood by working out explicitly the next interaction picture:[1] let us start with $i\hbar\partial_t|\psi_1(t)\rangle = H_1(t)|\psi_1(t)\rangle$ and treat it as if it were, formally, a Schrödinger equation. The diagonalization of $H_1(t)$ provides the eigenbasis $\{|n_1(t)\rangle\}$, $H_1(t)|n_1(t)\rangle = E_n^{(1)}(t)|n_1(t)\rangle$, which we fix again with the parallel transport condition, $\langle n_1(t)|\dot{n}_1(t)\rangle = 0$. A unitary operator $A_1 = \sum_n |n_1(t)\rangle\langle n_1(0)|$ plays now the same role as A_0 in the first (adiabatic) IP. It defines a second interaction picture wave function $|\psi_2(t)\rangle = A_1^\dagger(t)|\psi_1(t)\rangle$ that satisfies $i\hbar\partial_t|\psi_2(t)\rangle = H_2(t)|\psi_2(t)\rangle$, where $H_2(t) = A_1^\dagger(t)[H_1(t) - K_1(t)]A_1(t)$ and $K_1 = i\hbar\dot{A}_1A_1^\dagger$. If K_1 is zero or "small" enough, i.e., if a (first-order) superadiabatic approximation is valid, the dynamics would be uncoupled in the second interaction picture, namely,

$$|\psi_2(t)\rangle = U_2(t)|\psi_2(0)\rangle, \tag{4}$$

where

$$U_2(t) = \sum_n |n_1(0)\rangle e^{-\frac{i}{\hbar}\int_0^t E_n^{(1)}(t')dt'}\langle n_1(0)| \tag{5}$$

is the approximate evolution operator in the second IP for uncoupled motion. It may happen that a process is not adiabatic, since $K_0(t)$ may not be neglected, but (first-order) superadiabatic when $K_1(t)$ can be neglected. Transforming back to the Schrödinger picture, $|\psi_0^{(2)}(t)\rangle = A_0(t)A_1(t)U_2(t)|\psi_2(0)\rangle$ becomes

$$\left|\psi_0^{(2)}(t)\right\rangle = \sum_n\sum_m |m_0(t)\rangle\langle m_0(0)|n_1(t)\rangle e^{-\frac{i}{\hbar}\int_0^t E_n^{(1)}(t')dt'} \times \langle n_1(0)|\psi_0(0)\rangle, \tag{6}$$

and $|\psi_2(0)\rangle = |\psi_0(0)\rangle$ since $A_0(0) = A_1(0) = 1$. Garrido distinguished two different aspects [10]:

(i) Generalized adiabaticity: The evolution operator $A_0(t)A_1(t)U_2(t)$ provides an approximation to the actual (Schrödinger) dynamics up to a correction term of order $1/t_f^2$. This is so without imposing any boundary conditions (BCs) at $t = 0$ and $t = t_f$ on the Hamiltonian H_0.

(ii) Higher-order adiabaticity: $A_0(t)A_1(t)U_2(t)$ does not guarantee in general that $|n_0(0)\rangle$ evolves into $|n_0(t_f)\rangle$, up to a phase factor. If this is the objective, in other words, if a superadiabatic approximation should behave, at final times, like the adiabatic approximation, up to phase factors, then some BCs have to be imposed. Garrido discussed how generalized adiabaticity implies higher-order adiabaticity when BCs at the boundary times are imposed on the derivatives of H_0. [Garrido's distinction does not apply in [8], since there it is assumed from the start that all the derivatives of the Hamiltonian H_0 vanish at the (infinite) time edges.]

The second aspect is crucial to designing shortcuts to adiabaticity for finite process times using the superadiabatic iterative structure, so let us be more specific. First notice that Eq. (6) becomes exact if the term $A_1^\dagger K_1 A_1$ is added to the IP Hamiltonian, so that now the modified IP Hamiltonian is $H^{(2)} = H_2 + A_1^\dagger K_1 A_1 = A_1^\dagger H_1 A_1$. Then the modified SP Hamiltonian becomes $H_0^{(2)}(t) = H_0(t) + H_{\rm cd}^{(1)}(t)$, where $H_{\rm cd}^{(1)}(t) = A_0(t)K_1(t)A_0^\dagger(t)$. However, quite generally the populations of the final state (6) in the adiabatic basis $\{|n_0(t_f)\rangle\}$ will be different from those of the adiabatic process, unless (a) $\{|n_0(0)\rangle\} = \{|n_1(t_f)\rangle\}$, up to phase factors, and (b) $\{|n_0(0)\rangle\} = \{|n_1(0)\rangle\}$, also up to phase factors. (a) is satisfied when $K_0(t_f) = 0$. This makes $H_1(t_f)$ diagonal in the basis $\{|n_0(0)\rangle\}$ and $[H_1(t_f), H_0(0)] = 0$. (b) is satisfied when $K_0(0) = 0$, which implies $H_1(0) = H_0(0)$. In summary, the requirement is that the eigenstates of $H_1(t)$ at $t = 0$ and $t = t_f$ coincide with the eigenstates of $H_0(0)$. If, in addition, $K_1(0) = K_1(t_f) = 0$, not only the populations but also the initial and final Hamiltonians are the same for the "corrected" and for the reference processes, namely $H_0^{(2)}(0) = H_0(0)$ and $H_0^{(2)}(t_f) = H_0(t_f)$.

Further iterations define higher-order superadiabatic frames with IP equations $i\hbar\partial_t|\psi_j(t)\rangle = H_j|\psi_j(t)\rangle$, where

$$H_j = A_{j-1}^\dagger(H_{j-1} - K_{j-1})A_{j-1}, \tag{7}$$

$$K_j = i\hbar\dot{A}_jA_j^\dagger, \tag{8}$$

with $A_j(t) = \sum_n |n_j(t)\rangle\langle n_j(0)|$ and $H_j(t)|n_j(t)\rangle = E_n^{(j)}(t)|n_j(t)\rangle$. As the $A_j(0) = 1$ by construction, there is a common initial state $|\psi_j(0)\rangle = |\psi_0(0)\rangle$ for all iterations. The general form for the modified IP Hamiltonians is $H^{(j)} = H_j + A_{j-1}^\dagger K_{j-1}A_{j-1} = A_{j-1}^\dagger H_{j-1}A_{j-1}$. Thus, the form of the modified Hamiltonians in the SP is

$$H_0^{(j)} = H_0 + H_{\rm cd}^{(j-1)}, \tag{9}$$

where the SP counterdiabatic term is

$$H_{\rm cd}^{(j)} = B_jK_jB_j^\dagger = i\hbar B_j\dot{A}_jA_j^\dagger B_j^\dagger, \tag{10}$$

with $B_j = A_0\cdots A_{j-1}$ and $B_0 = I$. If $K_{j-1}(t)$ is small or negligible, $H_j(t)$ becomes diagonal in the basis $\{|n_{j-1}(0)\rangle\}$ and the IP equation becomes an uncoupled system with solutions $|\psi_j(t)\rangle = U_j(t)|\psi_j(0)\rangle$, where

$$U_j(t) = \sum_n |n_{j-1}(0)\rangle e^{-\frac{i}{\hbar}\int_0^t E_n^{(j-1)}(t')dt'}\langle n_{j-1}(0)| \tag{11}$$

is the approximate evolution operator in the jth IP. Correspondingly, the approximate solution in the SP is given by $|\psi_0^{(j)}(t)\rangle = A_0(t)A_1(t)\cdots A_{j-1}(t)U_j(t)|\psi_0(0)\rangle$. This solution becomes exact if the $H_{\rm cd}^{(j-1)}$ term is added to H_0, where in general the populations of $|\psi_0^{(j)}(t_f)\rangle$ in the adiabatic basis $\{|n_0(t_f)\rangle\}$ will be different from those of the adiabatic process, unless appropriate BCs are imposed. These boundary conditions are made explicit in the next section, and correspond partially to the conditions discussed by Garrido in [10] to define "higher-order adiabaticity."

Is there any advantage to using one or another counterdiabatic scheme? There are several reasons that could make

[1]The first IP and iteration just described, with dynamics governed by $H_1(t)$, generates the modified dynamics based on $H_0^{(1)}$ in the SP. This iteration may be naturally termed "adiabatic" since the unitary transformation used, A_0, relies on the usual adiabatic basis. Moreover, this is the IP used to perform the adiabatic approximation by neglecting K_0. The second iteration may be considered as the first "superadiabatic" one.

higher-order schemes attractive in practice: one is that the structure of the $H_{\rm cd}^{(j)}$ may change with j. For example, for a two-level atom population inversion problem, $H_{\rm cd}^{(0)} = \hbar(\dot\Theta_0/2)\sigma_y$, whereas $H_{\rm cd}^{(1)} = \hbar(\dot\Theta_1/2)(\cos\Theta_0\sigma_x - \sin\Theta_0\sigma_z)$, where the Θ_j are the polar angles corresponding to the Cartesian components of the Hamiltonian H_j, and the σ_u, with $u = x,y,z$, are Pauli matrices [4]. (We shall use the Cartesian decomposition $X\sigma_x + Y\sigma_y + Z\sigma_z$ for different Hamiltonians below.)

A second reason is that, for a fixed process time, the cd terms tend to be smaller in norm as j increases, up to a value in which they begin to grow [18]. An optimal iteration may thus be set [14,18]. The "asymptotic character" of the superadiabatic coupling terms and the eventual divergence of the sequence can be traced back to the existence of nonadiabatic transitions, even if they are small [8].

To generate shortcuts, one should pay attention not only to the size of the cd terms but also to the feasibility or approximate fulfillment of the required BCs at the boundary times. Thus, it may happen that an "optimal iteration," of minimal norm for the cd term, fails to provide a shortcut because of the BCs, as illustrated below in Sec. IV.

II. BOUNDARY CONDITIONS FOR SHORTCUTS TO ADIABATICITY VIA SUPERADIABATIC ITERATIONS

In this section, we set the boundary conditions that guarantee that $H_0^{(j)}(t)$ provides a shortcut to adiabaticity. We have seen that for $j = 1$ no conditions are required. For $j = 2$ we need that $\{|n_1(t_f)\rangle\} = \{|n_0(0)\rangle\}$ and $\{|n_1(0)\rangle\} = \{|n_0(0)\rangle\}$ (as before in these and similar expressions in brackets, the equalities should be understood up to phase factors), i.e., $K_0(t_f) = K_0(0) = 0$. For the iterations $j > 2$ we need that (a) $\{|n_{j-1}(0)\rangle\} = \{|n_0(0)\rangle\}$, which occurs when $K_{j-2}(0) = K_{j-3}(0) = \cdots = K_1(0) = K_0(0) = 0$ and (b) $\{|n_{j-1}(t_f)\rangle\} = \{|n_{j-2}(0)\rangle\}$, $\{|n_{j-2}(t_f)\rangle\} = \{|n_{j-3}(0)\rangle\}$, $\{|n_{j-3}(t_f)\rangle\} = \{|n_{j-4}(0)\rangle\}$, . . ., and $\{|n_1(t_f)\rangle\} = \{|n_0(0)\rangle\}$. This amounts to imposing $K_{j-2}(t_f) = K_{j-3}(t_f) = \cdots = K_1(t_f) = K_0(t_f) = 0$. The vanishing of $K_{j'}(0)$ for $j' \leqslant j-2$ implies that $H_0(0) = H_1(0) = \cdots = H_{j-1}(0)$, so (a) and (b) combined may be summarized as $\{|n_{j'}(0)\rangle\} = \{|n_{j'}(t_f)\rangle\} = \{|n_0(0)\rangle\}$ for all $j' \leqslant j-1$. Garrido showed that canceling out the first lth time derivatives of $H_0(0)$ and $H_0(t_f)$ makes $K_j(0) = 0$ and $K_j(t_f) = 0$ for $j = 1,\ldots,l-1$, respectively [10]. However, canceling out the derivatives of H_0 is a sufficient but not a necessary condition to cancel the coupling terms, so we find it more useful to focus instead on the coincidence of the bases. This is exemplified in Sec. IV.

III. ALTERNATIVE FRAMEWORK WITH A CONSTANT BASIS

An alternative to the formal framework described so far provides computational advantages. It was implicitly applied by Demirplak and Rice for a two-level system [7]. We shall generalize here and formulate this approach explicitly. We shall also show its essential equivalence to the former. The main idea is to use instead of the A_j a different set of unitary operators, $\tilde A_j(t) = \sum_n |\tilde n_j(t)\rangle\langle n|$, to define the sequence of interaction pictures, where $|\tilde n_j(t)\rangle$ are eigenstates of the new IP Hamiltonians $\tilde H_j(t)$, such that $\tilde H_j(t)|\tilde n_j(t)\rangle = \tilde E_n^{(j)}(t)|\tilde n_j(t)\rangle$, and $\{|n\rangle\}$ is a constant orthonormal basis *equal for all* j, which in principle does not necessarily coincide with $|n_j(0)\rangle$. Similarly to Eq. (7),

$$\tilde H_j = \tilde A_{j-1}^\dagger(\tilde H_{j-1} - \tilde K_{j-1})\tilde A_{j-1}, \tag{12}$$

where $\tilde K_j = i\hbar\dot{\tilde A}_j\tilde A_j^\dagger = i\hbar\sum_n |\dot{\tilde n}_j(t)\rangle\langle\tilde n_j(t)|$. The counterdiabatic terms in the SP are introduced as before, $\tilde H_{\rm cd}^{(j)} = \tilde B_j\tilde K_j\tilde B_j^\dagger$, where $\tilde B_j = \tilde A_0\cdots\tilde A_{j-1}$ with $\tilde B_0 = I$. We shall next show that these cd terms are independent of the chosen constant basis, so that $\tilde H_{\rm cd}^{(j)}(t) = H_{\rm cd}^{(j)}(t)$. Therefore, it is worth using $\tilde A_j(t)$ instead of $A_j(t)$ since they are simpler operators and significantly facilitate the manipulations as a common basis is used.

Let us start with the first iteration. Since $\tilde H_0(t) = H_0(t)$, then $\tilde E_n^{(0)}(t) = E_n^{(0)}(t)$, $|\tilde n_0(t)\rangle = |n_0(t)\rangle$, and $\tilde K_0 = K_0$, so $\tilde H_{\rm cd}^{(0)} = H_{\rm cd}^{(0)}$. In addition, from Eq. (7), $H_0 - K_0 = A_0H_1A_0^\dagger$, and substituting it in Eq. (12) leads to

$$\tilde H_1 = u_0H_1u_0^\dagger, \tag{13}$$

where we have defined a constant unitary operator

$$u_0 = \tilde A_0^\dagger A_0 = \sum_n |n\rangle\langle n_0(0)|,$$

$$\dot u_0 = 0.$$

Using

$$H_j(t) = \sum_n |n_j(t)\rangle E_n^{(j)}(t)\langle n_j(t)| \tag{14}$$

and

$$\tilde H_j(t) = \sum_n |\tilde n_j(t)\rangle \tilde E_n^{(j)}(t)\langle\tilde n_j(t)| \tag{15}$$

for $j = 1$ in Eq. (13), we get that $\tilde E_n^{(1)}(t) = E_n^{(1)}(t)$ and $|\tilde n_1(t)\rangle = u_0|n_1(t)\rangle$, while $|n\rangle = u_0|n_0(0)\rangle$. Expanding $\tilde H_{\rm cd}^{(1)} = \tilde A_0\tilde K_1\tilde A_0^\dagger$, we have that

$$\tilde H_{\rm cd}^{(1)}(t) = i\hbar\sum_{n,m,l,p} |\tilde n_0(t)\rangle\langle n|\dot{\tilde m}_1(t)\rangle\langle m|l\rangle\langle\tilde l_1(t)|p\rangle\langle\tilde p_0(t)|.$$

Using now $\langle m|l\rangle = \delta_{ml}$, $|\tilde n_0(t)\rangle = |n_0(t)\rangle$, $|n\rangle = u_0|n_0(0)\rangle$, and $|\tilde n_1(t)\rangle = u_0|n_1(t)\rangle$, it follows that $\tilde H_{\rm cd}^{(1)} = H_{\rm cd}^{(1)}$. Also, $\tilde K_1 = \tilde A_0^\dagger A_0K_1A_0^\dagger\tilde A_0 = u_0K_1u_0^\dagger$.

Repeating these steps for $j \geqslant 1$, $\tilde H_j = u_{j-1}H_ju_{j-1}^\dagger$ and $\tilde K_j = u_{j-1}K_ju_{j-1}^\dagger$, where

$$u_j = \tilde A_j^\dagger u_{j-1}A_j = \sum_n |n\rangle\langle n_j(0)|,$$

$$\dot u_j = 0.$$

This leads to $\tilde E_n^{(j)}(t) = E_n^{(j)}(t)$, $|\tilde n_j(t)\rangle = u_{j-1}|n_j(t)\rangle$, and $|n\rangle = u_{j-1}|n_{j-1}(0)\rangle$. Thus, for all $j \geqslant 0$,

$$\tilde H_{\rm cd}^{(j)} = H_{\rm cd}^{(j)}.$$

The boundary conditions to achieve shortcuts to adiabaticity take the same form as for the original framework in the previous section. Since $\tilde K_0 = K_0$ and $\tilde K_j = u_{j-1}K_ju_{j-1}^\dagger$ for

$j \geqslant 1$, for the jth iteration, with $j > 1$, we need that $\tilde{K}_0(0) = \tilde{K}_1(0) = \cdots = \tilde{K}_{j-2}(0) = 0$ and $\tilde{K}_0(t_f) = \tilde{K}_1(t_f) = \cdots = \tilde{K}_{j-2}(t_f) = 0$. Let us recall that no conditions were required for $j = 1$, although, as shown in the next section, using a convenient (constant or initial adiabatic) basis for specific Hamiltonians may also lead to conditions for $j = 1$.

IV. TWO-LEVEL ATOM

The general formalism will now be applied to the two-level atom. Assuming a semiclassical interaction between a laser electric field and the atom, the electric dipole, and the rotating wave approximations, the Hamiltonian of the system in a laser-adapted IP (that plays the role of the Schrödinger picture of the previous section) is

$$H_0(t) = \frac{\hbar}{2}\begin{pmatrix} -\Delta(t) & \Omega_R(t) \\ \Omega_R(t) & \Delta(t) \end{pmatrix}, \tag{16}$$

where $\Omega_R(t)$ is the Rabi frequency, assumed real, and $\Delta(t)$ is the detuning, in the "bare basis" of the two-level system, $|1\rangle = \binom{1}{0}$, $|2\rangle = \binom{0}{1}$. The Hamiltonians of the consecutive interaction pictures can be written as [7]

$$\tilde{H}_j(t) = \begin{pmatrix} Z_j(t) & X_j(t) - iY_j(t) \\ X_j(t) + iY_j(t) & -Z_j(t) \end{pmatrix}, \tag{17}$$

or $\tilde{H}_j = X_j\sigma_x + Y_j\sigma_y + Z_j\sigma_z$ [4]. Then, $X_0(t) = \hbar\Omega_R(t)/2$, $Y_0(t) = 0$, and $Z_0(t) = -\hbar\Delta(t)/2$. X_j, Y_j, and Z_j are the Cartesian coordinates of the "trajectory" of $\tilde{H}_j(t)$. It is also useful to consider the corresponding polar, azimuthal, and radial spherical coordinates, $\Theta_j(t)$, $\Phi_j(t)$, and $R_j(t)$ [4,7], that satisfy

$$\begin{aligned} \cos(\Theta_j) &= \frac{Z_j}{R_j}, \quad \sin(\Theta_j) = \frac{P_j}{R_j}, \quad 0 \leqslant \Theta_j \leqslant \pi, \\ \cos(\Phi_j) &= \frac{X_j}{P_j}, \quad \sin(\Phi_j) = \frac{Y_j}{P_j}, \quad 0 \leqslant \Phi_j \leqslant 2\pi, \end{aligned} \tag{18}$$

with $R_j = \sqrt{X_j^2 + Y_j^2 + Z_j^2}$ and $P_j = \sqrt{X_j^2 + Y_j^2}$, where the positive branch is taken. The eigenvalues of $\tilde{H}_j(t)$ are $E_1^{(j)} = -R_j$ and $E_2^{(j)} = R_j$, and the corresponding eigenstates $\{|\tilde{n}_j(t)\rangle\}$ are

$$\begin{aligned} |\tilde{1}_j\rangle &= e^{i\varepsilon_j}\left[e^{-i\Phi_j/2}\sin\left(\frac{\Theta_j}{2}\right)|1\rangle - e^{i\Phi_j/2}\cos\left(\frac{\Theta_j}{2}\right)|2\rangle\right], \\ |\tilde{2}_j\rangle &= e^{-i\varepsilon_j}\left[e^{-i\Phi_j/2}\cos\left(\frac{\Theta_j}{2}\right)|1\rangle + e^{i\Phi_j/2}\sin\left(\frac{\Theta_j}{2}\right)|2\rangle\right], \end{aligned} \tag{19}$$

where the phase

$$\varepsilon_j(t) = -\frac{1}{2}\int_0^t \dot{\Phi}_j(t')\cos\left[\Theta_j(t')\right]dt' \tag{20}$$

is introduced to fulfill the parallel transport condition $\langle\tilde{n}_j|\dot{\tilde{n}}_j\rangle = 0$. We define $\tilde{A}_j = |\tilde{1}_j(t)\rangle\langle 1| + |\tilde{2}_j(t)\rangle\langle 2|$. The matrix $\tilde{A}_j(t)$ under these conditions is

$$\tilde{A}_j = \begin{pmatrix} \sin\left(\frac{\Theta_j}{2}\right)e^{i\varepsilon_j - i\Phi_j/2} & \cos\left(\frac{\Theta_j}{2}\right)e^{-i\varepsilon_j - i\Phi_j/2} \\ -\cos\left(\frac{\Theta_j}{2}\right)e^{i\varepsilon_j + i\Phi_j/2} & \sin\left(\frac{\Theta_j}{2}\right)e^{-i\varepsilon_j + i\Phi_j/2} \end{pmatrix}. \tag{21}$$

Then, from Eq. (8),

$$\begin{aligned} \tilde{K}_j = {} & \frac{\hbar}{2}\left[-\dot{\Theta}_j\sin(\Phi_j) - \frac{\dot{\Phi}_j}{2}\cos(\Phi_j)\sin(2\Theta_j)\right]\sigma_x \\ & + \frac{\hbar}{2}\left[\dot{\Theta}_j\cos(\Phi_j) - \frac{\dot{\Phi}_j}{2}\sin(\Phi_j)\sin(2\Theta_j)\right]\sigma_y \\ & + \frac{\hbar\dot{\Phi}_j}{2}\sin^2(\Theta_j)\sigma_z. \end{aligned} \tag{22}$$

Note that $\tilde{A}_j^\dagger\tilde{K}_j\tilde{A}_j = \tilde{A}_j^\dagger\dot{\tilde{A}}_j$ has only nondiagonal elements in the bare basis $\{|1\rangle, |2\rangle\}$ [7].

From Eq. (7), the Cartesian coordinates of $\tilde{H}_{j+1}(t)$ are

$$\begin{aligned} X_{j+1} &= \frac{\hbar}{2}[\dot{\Theta}_j\sin(2\varepsilon_j) - \dot{\Phi}_j\sin(\Theta_j)\cos(2\varepsilon_j)], \\ Y_{j+1} &= \frac{\hbar}{2}[-\dot{\Theta}_j\cos(2\varepsilon_j) - \dot{\Phi}_j\sin(\Theta_j)\sin(2\varepsilon_j)], \\ Z_{j+1} &= -R_j. \end{aligned} \tag{23}$$

In general, if $\Phi_j(t)$ is constant for a particular $j = J$, then $\dot{\Phi}_J(t) = 0$, and from Eq. (20), $\varepsilon_J(t) = 0$. Thus, taking into account Eq. (23), we have that $X_{J+1}(t) = 0$ and $Y_{J+1}(t) = -\hbar\dot{\Theta}_J/2$. Equation (18) leads to $\Phi_{J+1}(t) = \{\pi/2, 3\pi/2\}$, with $\pi/2$ when $Y_{J+1} > 0$ ($\dot{\Theta}_J < 0$), and $3\pi/2$ when $Y_{J+1} < 0$ ($\dot{\Theta}_J > 0$). If $Y_{J+1} = 0$, Φ_{J+1} is discontinuous and $\Theta_{J+1} = \pi$. Therefore, $\varepsilon_{J+1}(t) = \{0, \pm\pi/2\}$. From here, several general conditions can be deduced for $j' > J$: $\Phi_{j'>J}(t) = \{\pi/2, 3\pi/2\}$, $\varepsilon_{j'>J}(t) = \{0, \pm\pi/2\}$, $X_{j'>J}(t) = 0$, and $Y_{J+1}(t) = -\hbar\dot{\Theta}_J/2$ or $Y_{j'>J+1}(t) = \pm\hbar\dot{\Theta}_{j'-1}/2$. Moreover, from Eq. (22), $\tilde{K}_{j'>J} = \pm(\hbar\dot{\Theta}_{j'}/2)\sigma_x$ with positive sign if $\Phi_{j'}(t) = 3\pi/2$ and negative sign if $\Phi_{j'}(t) = \pi/2$. Equation (18) and $Y_0(t) = 0$ imply $\Phi_0(t) = 0$ if $X_0(t) > 0$ and $\Phi_0(t) = \pi$ if $X_0(t) < 0$. We may thus take $J = 0$ and apply the above relations, for example $\dot{\Phi}_0(t) = 0$ and $\varepsilon_0(t) = 0$.[2]

As we mentioned before, the method fails as a shortcut to adiabaticity when the boundary conditions are not well fulfilled. To have a shortcut generated by the iteration j, we require that $\Delta(t)$ and $\Omega_R(t)$ are such that

$$|\tilde{1}_{j'}(0)\rangle \approx |1\rangle, \quad |\tilde{2}_{j'}(0)\rangle \approx |2\rangle, \tag{24}$$

$$|\tilde{1}_{j'}(t_f)\rangle \approx |1\rangle, \quad |\tilde{2}_{j'}(t_f)\rangle \approx |2\rangle \tag{25}$$

for $0 < j' < j$, up to phase factors. For $j' = 0$, a natural and simple assumption is that the bare basis coincides initially with the adiabatic basis, i.e., Eq. (24); at t_f we assume that the bare and adiabatic bases also coincide, allowing for permutations in the indices and phase factors.

At $t = 0$, using Eq. (19), taking into account that, from Eq. (20), $\varepsilon_{j'}(0) = 0$, and that $\Phi_0(t) = 0$, $\sin[\Theta_{j'}(0)/2] = 1$ and $\cos[\Theta_{j'}(0)/2] = 0$ are required, or $\Theta_{j'}(0) = \pi$. Then, $\cos[\Theta_{j'}(0)] = Z_{j'}(0)/R_{j'}(0) = -1$. This condition is fulfilled if

$$Z_{j'}^2(0) \gg X_{j'}^2(0) + Y_{j'}^2(0) \tag{26}$$

as long as $Z_{j'=0}(0) < 0$, and knowing that $Z_{j'>0}(t) = -R_{j'-1}(t) < 0$. The condition (26) can be simplified for

[2]The analysis in this paragraph follows closely [7], but some of the results differ, in particular the values allowed for the phases $\varepsilon_{j'>J}$.

specific j' values as

$$|Z_0(0)| \gg |X_0(0)|, \tag{27}$$

$$|Z_{j'>0}(0)| \gg |Y_{j'>0}(0)|. \tag{28}$$

At $t = t_f$,

$$Z_{j'}^2(t_f) \gg X_{j'}^2(t_f) + Y_{j'}^2(t_f) \tag{29}$$

should be satisfied, where now, $\Theta_0(t_f)$ can be either 0 if $Z_0(t_f) > 0$ or π if $Z_0(t_f) < 0$, and $\Theta_{j'>0}(t_f) = \pi$. As before, this condition splits into

$$|Z_0(t_f)| \gg |X_0(t_f)|, \tag{30}$$

$$|Z_{j'>0}(t_f)| \gg |Y_{j'>0}(t_f)|. \tag{31}$$

As an example, we consider now a Landau-Zener scheme for H_0 (for the Allen-Eberly scheme we have found similar results), and we study the behavior of $H_0^{(j)}$ with $j = 1$, 2, 3, and 4, and the populations of the bare states driven by these Hamiltonians.

For the Landau-Zener model, $\Delta(t)$ is linear in time and $\Omega_R(t)$ is constant,

$$\begin{aligned} \Delta_{lz}(t) &= \alpha(t - t_f/2), \\ \Omega_{R,lz}(t) &= \Omega_{0,lz}, \end{aligned} \tag{32}$$

where α is the chirp and $\Omega_{0,lz}$ is a constant Rabi frequency. Condition (27) can be restated as

$$t_f \gg 2\left|\frac{\Omega_{0,lz}}{\alpha}\right|. \tag{33}$$

We consider the parameters $\alpha = -20$ MHz^2, $\Omega_{0,lz} = 0.2$ MHz, and $t_f = 0.2$ μs for which the dynamics with H_0 is nonadiabatic, see the Appendix A. Figure 1 shows X, Y, and Z components of H_0 and $H_0^{(j)}$, with $j = 1$, 2, 3, and 4. In Figs. 1(a) and 1(b) and in Table I we see that $H_0^{(2)}$ (corresponding to the first superadiabatic iteration) is optimal with respect to applied intensities. Moreover, it cancels the Y component completely, which is a simplifying practical advantage in some realizations of the two-level system [4,11]. From the second superadiabatic iteration, both intensities start to increase again. For the parameters above, condition (33) is satisfied since $t_f = 20 \times |\Omega_{0,lz}/\alpha|$, but not so condition (28). Figure 1 shows the disagreement between $H_0^{(j)}$ and H_0, at $t = 0$ and $t = t_f$ for $j > 1$. Figure 2 shows that only $H_0^{(1)} = H_0 + H_{\rm cd}^{(0)}$ inverts the population of $|1\rangle$, $P_1(t)$, whereas the rest of the Hamiltonians fail to do so.

TABLE I. Maxima of the X and Y components of H_0 and $H_0^{(j)}$ for $j = 1$, 2, 3, 4, and 5. Parameters: $\alpha = -20$ MHz^2, $\Omega_{0,lz} = 0.2$ MHz, and $t_f = 0.2$ μs.

Hamiltonian	$\lvert X_{\max}\rvert/\hbar$ (MHz)	$\lvert Y_{\max}\rvert/\hbar$ (MHz)
$H_0/\hbar$	0.1	0
$H_0^{(1)}/\hbar$	0.1	49.9
$H_0^{(2)}/\hbar$	10	0
$H_0^{(3)}/\hbar$	8.4	2.8
$H_0^{(4)}/\hbar$	46.8	28.1
$H_0^{(5)}/\hbar$	56.2	62.8

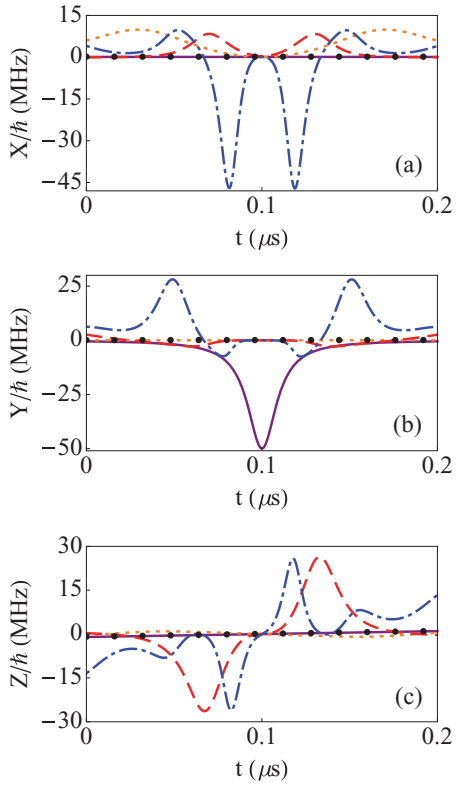

FIG. 1. (Color online) The (a) X, (b) Y, and (c) Z components for the Landau-Zener scheme, of $H_0(t)$ (black dots), $H_0^{(1)}$ (purple solid line), $H_0^{(2)}$ (orange dotted line), $H_0^{(3)}$ (red dashed line), and $H_0^{(4)}$ (blue dot-dashed line). In (a) and (c) the black dots and the purple solid line coincide and in (b) the black dots coincide with the orange dotted line. Parameters: $\alpha = -20$ MHz^2, $\Omega_{0,lz} = 0.2$ MHz, and $t_f = 0.2$ μs.

V. DISCUSSION

In this paper, we have investigated the use of quantum superadiabatic iterations (a nonconvergent sequence of nested interaction pictures) to produce shortcuts to adiabaticity. Each superadiabatic iteration may be used in two ways: (i) to generate a superadiabatic approximation to the dynamics, or (ii) to generate a counterdiabatic term that, when added to the original Hamiltonian, makes the approximate dynamics

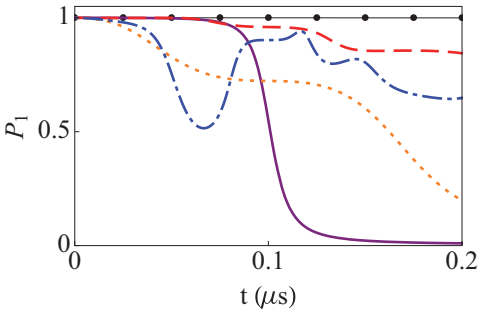

FIG. 2. (Color online) Population of the state $|1\rangle$, $P_1(t)$, for the Hamiltonians $H_0(t)$ (black solid line with dots), $H_0^{(1)}$ (purple solid line), $H_0^{(2)}$ (orange dotted line), $H_0^{(3)}$ (red dashed line), and $H_0^{(4)}$ (blue dot-dashed line), with the Landau-Zener scheme. Parameters as in Fig. 1: $\alpha = -20$ MHz^2, $\Omega_{0,lz} = 0.2$ MHz, and $t_f = 0.2$ μs.

exact. The second approach, however, does not automatically generate shortcuts to adiabaticity, namely a Hamiltonian that produces in a finite time the same final populations as the adiabatic dynamics. The boundary conditions needed for the second approach to generate a shortcut have been spelled out. This work is parallel to the investigation by Garrido to establish conditions so that the approach (i) provides an adiabatic-like approximation [10]. We have also described an alternative framework to the usual set of superadiabatic equations which offers some computational advantages, and we have applied the general formalism to the particular case of a two-level system. An optimal superadiabatic iteration with respect to the norm of the counterdiabatic term is not necessarily the best shortcut, or in fact a shortcut at all, because of the possible failure of the boundary conditions.

We end by mentioning further questions worth investigating on the superadiabatic framework as a shortcut-to-adiabaticity generator. For example, other operations different from the population control of two-level systems (such as transport or expansions of cold atoms) have to be studied. Unitary transformations may also be applied to simplify the Hamiltonian structure making use of symmetries [4]. They have been discussed before as a way to modify the first (adiabatic) iteration [4,14] and applied to perform a fast population inversion of a condensate in the bands of an optical lattice [11]. However, a systematic application and study, e.g., of the order with respect to the small (slowness) parameter, in particular for higher superadiabatic iterations, are still pending. A comparison with other methods to get shortcuts, at formal and practical levels, would be useful too. A preliminary step in this direction, relating and comparing the invariant-based inverse engineering approach to the counterdiabatic approach of the first (adiabatic) iteration, was presented in [22]; see also the Appendix B. Finally, comparisons among superadiabatic iterations themselves have to be performed, in particular regarding practical aspects such as the transient excitations involved [23].

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APPENDIX A: ADIABATICITY AND BOUNDARY CONDITIONS FOR THE LANDAU-ZENER PROTOCOL

The adiabaticity condition for a two-level atom driven by the Hamiltonian (16) is [24]

$$\tfrac{1}{2}|\Omega_a(t)| \ll |\Omega(t)|, \tag{A1}$$

where $\Omega_a(t) \equiv [\Omega_R(t)\dot{\Delta}(t) - \dot{\Omega}_R(t)\Delta(t)]/\Omega^2(t)$ and $\Omega = \sqrt{\Delta^2 + \Omega_R^2}$. For the Landau-Zener scheme, this condition takes the form

$$|\alpha| \ll 2\Omega_{0,lz}^2. \tag{A2}$$

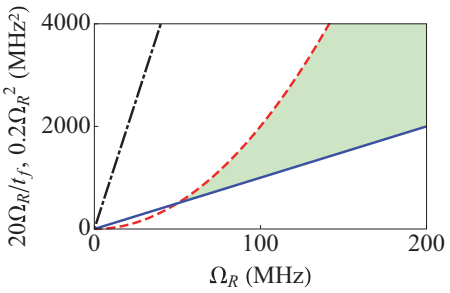

FIG. 3. (Color online) $0.2\Omega_{0,lz}^2$ (red dashed line) and $20|\Omega_{0,lz}|/t_f$ (blue dashed line for $t_f = 2$ μs and black dot-dashed line for $t_f = 0.2$ μs). The shaded (green) area corresponds to values of α satisfying $20|\Omega_{0,lz}|/t_f < |\alpha| < 0.2\Omega_{0,lz}^2$, namely, the process is adiabatic and the eigenstates at the boundary times are essentially the bare states. No such area exists for $t_f = 0.2$ μs in the domain shown.

The inequalities that α must satisfy so that the system is adiabatic and also fulfills the boundary condition (33) are

$$2|\Omega_{0,lz}|/t_f \ll |\alpha| \ll 2\Omega_{0,lz}^2. \tag{A3}$$

Figure 3 shows the (shaded area) region for which α satisfies $20|\Omega_{0,lz}|/t_f < |\alpha| < 0.2\Omega_{0,lz}^2$ when $t_f = 2$ μs. No such area exists in the depicted domain for $t_f = 0.2$ μs. For this shorter time, the critical point where $1/t_f = \Omega_{0,lz}/100$ corresponds to $\Omega_{0,lz} = 500$ MHz and detunings of up to 5 GHz. Both may be problematic, as very large laser intensities and detunings could excite other transitions.

APPENDIX B: INVARIANTS

The superadiabatic sequence may be pictured as an attempt to find a higher-order frame for which a coupling term K_j is zero in the dynamical equation so that there are no transitions in some basis. This would mean that the states that the system follows exactly have been found, in other words, the eigenvectors of a dynamical invariant $I(t)$ [22,25,26]. When counterdiabatic terms are added, it is easy to construct invariants for $H_0^{(j)}$ from the instantaneous eigenstates of $H_0(t)$. However, quite generally this is not enough to generate a shortcut to adiabaticity because the boundary conditions to perform a quasiadiabatic process (one that ends up with the same populations than the adiabatic one) may not be satisfied. A way out is to design the invariant first, and then $H(t)$ from it, satisfying the boundary conditions $[I(t), H(t)] = 0$ at $t = 0$ and $t = t_f$, and such that

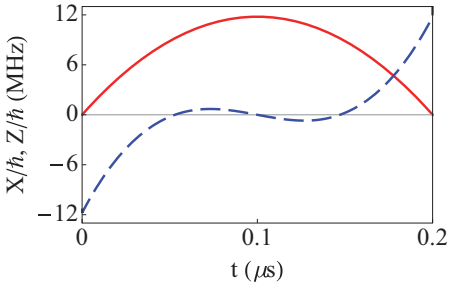

FIG. 4. (Color online) X (red solid line) and Z (blue dashed line) components of the Hamiltonian obtained using the invariant-based inverse engineering method. $t_f = 0.2$ μs.

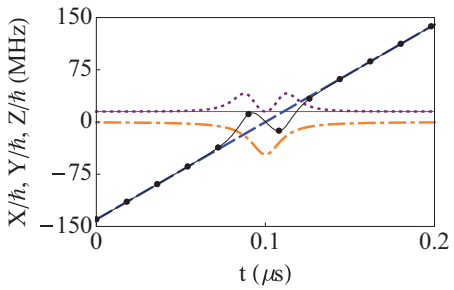

FIG. 5. (Color online) The components $X_0(t)$ (red solid line) and $Z_0(t)$ (blue dashed line) of $H_0(t)$, the $Y(t)$ component of $H_0^{(1)}(t)$ (orange dot-dashed line), and the $X(t)$ (purple dotted line) and $Z(t)$ (black solid line with dots) components of $H_0^{(2)}$, for the Landau-Zener scheme. Parameters: $\alpha = -2800$ MHz^2, $\Omega_{0,lz} = 30$ MHz, and $t_f = 0.2$ μs.

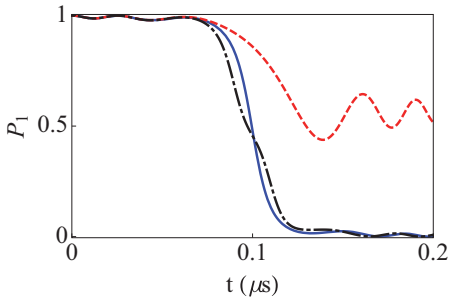

FIG. 6. (Color online) Population of $|1\rangle$, $P_1(t)$, for the Hamiltonians $H_0(t)$ (red dashed line), $H_0^{(1)}$ (blue solid line), and $H_0^{(2)}$ (black dot-dashed line), with the Landau-Zener scheme. Parameters as in Fig. 5: $\alpha = -2800$ MHz^2, $\Omega_{0,lz} = 30$ MHz, and $t_f = 0.2$ μs.

$H(0) = H_0(0)$ and $H(t_f) = H_0(t_f)$ [1,22]. For the general Hamiltonian in Eq. (16), a dynamical invariant of the corresponding Schrödinger equation may be parametrized as [22]

$$I(t) = \frac{\hbar}{2}\nu \begin{pmatrix} \cos\gamma(t) & \sin\gamma(t)e^{i\beta(t)} \\ \sin\gamma(t)e^{-i\beta(t)} & -\cos\gamma(t) \end{pmatrix}, \tag{B1}$$

where ν is an arbitrary constant with units of frequency to keep $I(t)$ with dimensions of energy. From the invariance condition for I,

$$\frac{dI(t)}{dt} \equiv \frac{\partial I(t)}{\partial t} - \frac{i}{\hbar}[I(t), H_0(t)] = 0, \tag{B2}$$

the functions $\gamma(t)$ and $\beta(t)$ must satisfy the differential equations

$$\begin{aligned} \dot{\gamma} &= \Omega_R \sin\beta, \\ \dot{\beta} &= \Delta + \Omega_R \cos\beta \cot\gamma. \end{aligned} \tag{B3}$$

To achieve a population inversion, the boundary values for γ should be $\gamma(0) = 0$ and $\gamma(t_f) = \pi$. Assuming a polynomial ansatz [22,27] for $\gamma(t)$ and $\beta(t)$, as $\gamma(t) = \sum_{n=0}^{3} a_n t^n$ with the boundary conditions $\gamma(0) = \pi$, $\gamma(t_f) = \dot{\gamma}(0) = \dot{\gamma}(t_f) = 0$, and $\beta(t) = \sum_{n=0}^{4} b_n t^n$ with the boundary conditions $\beta(0) = \beta(t_f/2) = \beta(t_f) = -\pi/2$, $\dot{\beta}(t_f) = -\pi/(2t_f)$, and $\dot{\beta}(0) = \pi/(2t_f)$, we can construct Δ and Ω_R [22]. These two functions are shown in Fig. 4, for $t_f = 0.2$ μs ($\Omega_R = 2X/\hbar$ and $\Delta = -2Z/\hbar$). For the same process time t_f we also plot in Fig. 5 $X_0(t)$ and $Z_0(t)$ for a Landau-Zener protocol in which the Rabi frequency is slightly larger than the maximum required for the invariant-based protocol: $\Omega_{0,lz} = 30$ MHz. As explained in the Appendix A, an unreasonably high laser intensity would be required to make it adiabatic while satisfying the bare-state condition at the edges, and $\Omega_{0,lz} = 30$ MHz is still too small to satisfy Eq. (A3). This is evident in the failure to invert the population, see Fig. 6. We use $\alpha = -2800$ MHz^2 to have the bare states as eigenvectors at the time edges which implies a rather large detuning. Figure 5 also depicts the $Y(t)$ component of $H_0^{(1)}$ and the $X(t)$ and $Z(t)$ components of $H_0^{(2)}$ for $t_f = 0.2$ μs. With these parameters these Hamiltonians provide shortcuts to adiabaticity, see Fig. 6, but they use very high detunings compared to those of the invariant-based protocol. This example does not mean, however, that invariant-based engineering is systematically more efficient. Invariant-based engineering and the counterdiabatic approach provide families of protocols that depend on the chosen interpolating auxiliary functions in the first case and on the reference Hamiltonian H_0 in the second. Their potential equivalence was studied in [22].

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