Inhibiting unwanted transitions in population transfer in two- and three-level quantum systems

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Abstract

We construct fast and stable control schemes for two- and three-level quantum systems. These schemes result in an almost perfect population transfer even in the presence of an additional, unwanted and uncontrollable transition. Such schemes are developed by first using the techniques of ‘shortcuts to adiabaticity’ and then introducing and examining a measure of the scheme’s sensitivity to an unwanted transition. We optimize the schemes to minimize this sensitivity and provide examples of shortcut schemes which lead to a nearly perfect population inversion even in the presence of unwanted transitions.

Keywords: population transfer, shortcuts to adiabaticity, quantum control

(Some figures may appear in colour only in the online journal)

1. Introduction

The manipulation of the state of a quantum system with time-dependent interacting fields is a fundamental operation in atomic and molecular physics. Modern applications of this quantum control such as quantum information processing [1, 2] require fast schemes with a high fidelity (typically with an error lower than $10^{-4}$ [1, 2]) which must also be very stable with respect to imperfections of the system or fluctuations of the control parameters.

Most methods used may be classified into two major groups: fast, resonant, fixed-area pulses, and slow adiabatic methods such as ‘rapid’ adiabatic passage. Fixed area pulses are traditionally considered to be fast but unstable with respect to perturbations. For two-level systems, an example of a fixed area pulse is a $\pi$ pulse. A $\pi$ pulse may be fast but is highly sensitive to variations in the pulse area and to inhomogeneities in the sample [3]. An alternative to a single $\pi$ pulse are composite pulses [4–6], which still need an accurate control of pulse phase and intensity. On the other hand, the canonical robust option is to perform operations adiabatically [7–9]. Nevertheless, such schemes are slow and therefore likely to be affected by decoherence or noise over the long times required and do not lead to an exact transfer.

A compromise is to use ‘shortcuts to adiabaticity’ (STA), which may be broadly defined as the processes that lead to the same final populations as the adiabatic approach but in a shorter time, for a review see [10, 11]. In particular, STA for two- and three-level systems are developed in [12–16] and [17] respectively.

Nonetheless, in an experimental implementation, noise and systematic error in the control parameters—i.e. calibration imperfections—can limit the ability to quickly and robustly manipulate the system. The stability and optimization of STA schemes in two-level systems versus amplitude noise and systematic error in the Rabi frequency has been studied in [14]; their stability versus dephasing noise and systematic frequency error has been studied and optimized in [15, 18] and the stability versus bit-flip noise has been studied in [11].

In an experimental implementation the system is also never an ideal two- or three-level system. There may be unwanted couplings to other levels.

In this paper, we develop STA inversion schemes which lead to nearly perfect population inversion even in the case of such unwanted uncontrollable transitions. To achieve this we examine the effect of unwanted couplings to STA in two- and three-level quantum systems and we develop STA schemes with minimal sensitivity to unwanted and uncontrollable
Here we will review the derivation of invariant-based shortcuts in two-level quantum systems leading to nearly perfect population inversion in the case of additional unwanted, uncontrollable transitions. Note that this is different from [19]; in that paper the effect of such unwanted transitions for composite pulses has been examined and optimized where it was also assumed that the phase of the unwanted coupling to another level could be controlled in a time-dependent way.

The remainder of this paper is structured as follows. In the subsequent section, we briefly review STA for two-level systems. In section 3, we examine the sensitivity of STA schemes to unwanted transitions and develop schemes to minimize this sensitivity (which leads to nearly perfect population inversion for these schemes). In section 4, we review STA for three-level systems. We examine their sensitivity to unwanted transitions in section 5 and we also develop schemes in the three-level case leading to nearly perfect population inversion in the case of additional unwanted, uncontrollable transitions.

2. Invariant-based shortcuts in two-level quantum systems

Here we will review the derivation of invariant-based STA schemes in two-level quantum systems following the explanation given in [14]. We assume our two-level system (see also figure 1(a)) has a Hamiltonian of the form

\[ H_{2L}(t) = \frac{\hbar}{2} \left( \begin{array}{cc} -\delta_2(t) & \Omega_R(t) - i\Omega_L(t) \\ \Omega_R(t) + i\Omega_L(t) & \delta_2(t) \end{array} \right) \]

expressed in the ‘bare basis’ of the two-level system

\[ |1\rangle = \left( \begin{array}{c} 1 \\ 0 \end{array} \right) \quad \text{and} \quad |2\rangle = \left( \begin{array}{c} 0 \\ 1 \end{array} \right). \]

We also assume \( \delta_2(t) = \Omega_R(t) = \Omega_L(t) = 0 \) for \( t < 0 \) and for \( t > T \).

An example of such a quantum system would be a semi-classical coupling of two atomic levels with a laser in a laser-adapted interaction picture (using the dipole and rotating-wave approximations). In this setting, \(|1\rangle\) might represent the ground state and \(|2\rangle\) a meta-stable excited state of the atom. \( \Omega(t) = \Omega_R(t) + i\Omega_L(t) \) would be the complex Rabi frequency (where \( \Omega_R \) and \( \Omega_L \) are the real and imaginary parts) and \( \delta_2 \) would be the time-dependent detuning between transition and laser frequencies. The Rabi frequency is given by \( \Omega = \mu \mathcal{E} / \hbar \) where \( \mu \) is the (in general complex) transition dipole moment. The electric field at the position of the atom is given by \( \mathcal{E} = \text{Re}(\mathcal{E}_0 e^{-i\omega t}) \) where \( \mathcal{E}_0 = \mathcal{E}_1 \mathcal{E}_0 \) is the amplitude of the electric field with \( \mathcal{E} \) being the unit polarization vector of the electric field (which is for example complex in the case of circular polarized light). Therefore, in general, the Rabi frequency might be complex and its real and imaginary part might be controlled by controlling polarization and amplitude of the laser. Even with a complex Rabi frequency, the Hamiltonian \( (1) \) is still Hermitian and describes a closed quantum system with coherent evolution and no dissipation.

To simplify the language we will assume this setting for convenience in the following, noting that our reasoning will still pertain to any other two-level system such as for example the spin dynamics in a quantum dot [20] or a Bose–Einstein condensate on an accelerated optical lattice [21]. In other settings, \( \Omega(t) \) and \( \delta_2(t) \) will correspond to different physical quantities.

The goal is to achieve perfect population inversion in a short time in a two-level quantum system. The system should start at \( t = 0 \) in state \(|1\rangle\) and end in state \(|2\rangle\) (up to a phase) at final time \( T \). In order to design a scheme to achieve this goal i.e. to design a STA, we make use of Lewis–Riesenfeld invariants [22]. A Lewis–Riesenfeld invariant of \( H_{2L} \) is a Hermitian operator \( I(t) \) such that

\[ \frac{\partial I}{\partial t} + i \hbar [H_{2L}, I] = 0. \]

In this case \( I(t) \) is given by

\[ I(t) = \frac{\hbar}{2} \mu \left( \begin{array}{cc} \cos (\theta(t)) & \sin (\theta(t)) e^{-i\omega(t)} \\ \sin (\theta(t)) e^{i\omega(t)} & -\cos (\theta(t)) \end{array} \right) \]

where \( \mu \) is an arbitrary constant with units of frequency to keep \( I(t) \) with dimensions of energy. The functions \( \theta(t) \) and \( \alpha(t) \) must satisfy the following equations:

\[ \dot{\theta} = \Omega_L \cos \alpha - \Omega_R \sin \alpha, \]

\[ \dot{\alpha} = -\delta_2 - \cot \theta (\Omega_R \cos \alpha + \Omega_L \sin \alpha). \]

The eigenvectors of \( I(t) \) are

\[ |\phi_+(t)\rangle = \left( \begin{array}{c} \cos (\theta/2) e^{-i\alpha/2} \\ \sin (\theta/2) e^{i\alpha/2} \end{array} \right), \]

\[ |\phi_-(t)\rangle = \left( \begin{array}{c} \sin (\theta/2) e^{-i\alpha/2} \\ -\cos (\theta/2) e^{i\alpha/2} \end{array} \right) \]

with eigenvalues \( \pm \hbar \mu. \) One can write a general solution of the Schrödinger equation

\[ i\hbar \frac{d}{dt} |\Psi(t)\rangle = H_{2L}(t) |\Psi(t)\rangle \]

as a linear combination of the eigenvectors of \( I(t) \) i.e.

\[ |\Psi(t)\rangle = c_+ e^{i\kappa_+(t)} |\phi_+(t)\rangle + c_- e^{i\kappa_-(t)} |\phi_-(t)\rangle \]

where \( c_\pm \in \mathbb{C} \) and \( \kappa_\pm(t) \) are the Lewis–Riesenfeld phases [22]

\[ \kappa_\pm(t) = \frac{\hbar}{\mu} \langle \phi_\pm(t) | (i\hbar \delta_2 - H_{2L}(t)) | \phi_\pm(t) \rangle. \]
Therefore, it is possible to construct a solution
\[ |\psi(t)\rangle = |\phi_v(t)\rangle e^{-i\theta t}/2 \] 
(11)
where \( \gamma = \pm 2k_\theta \). From (10) we get
\[ \dot{\gamma} = \frac{1}{\sin \theta} (\Omega_R \cos \alpha + \Omega_J \sin \alpha) . \] 
(12)
For population inversion it must be the case that \( \theta(0) = 0 \) and \( \theta(T) = \pi \). This ensures that \( |\psi(0)\rangle = |1\rangle \) and \( |\psi(T)\rangle = |2\rangle \) up to a phase. Note, that this method is not limited to going from state |1\rangle to state |2\rangle; the initial and final states can be determined by changing the boundary conditions on \( \theta \) and \( \alpha \).

Using equations (5), (6) and (12) we can retrieve the physical quantities:
\[ \Omega_R = \cos \alpha \sin \theta \dot{\gamma} - \sin \alpha \dot{\theta} , \] 
(13)
\[ \Omega_J = \sin \alpha \sin \theta \dot{\gamma} + \cos \alpha \dot{\theta} , \] 
(14)
\[ \delta_3 = -\cos \theta \dot{\gamma} - \dot{\alpha} . \] 
(15)
From this we can see that if the functions \( \alpha, \gamma, \) and \( \theta \) are chosen with the appropriate boundary conditions, perfect population inversion would be achieved at a time \( T \) assuming no perturbation or unwanted transitions. These functions will henceforth be referred to as ancillary functions.

We are considering here the general case of a complex Rabi frequency. Nevertheless, one could easily add the additional constraint that the Rabi frequency should be real (i.e. \( \Omega_R = 0 \) where \( \Omega_J \) is given by equation (14)) if this might be required by the specific physical two-level system. In fact, the optimized schemes which we will derive below will have a real Rabi frequency. In the following section we assume that there is an additional unwanted coupling to a third level.

3. Two-level quantum system with unwanted transition

3.1. Model
We assume there are in fact three levels in the atom as shown in figure 1(b) and the energy of level \( \nu \) is \( \hbar \omega _\nu \) where \( \nu = 1, 2, 3 \). Without loss of generality we set \( \omega_3 = 0 \). The frequency of the laser coupling levels |1\rangle and |2\rangle is denoted by \( \omega _L \). The detuning with the second level is given by
\[ \delta_2 = \omega_2 - \omega _L . \] 
(16)
We assume that this laser is also unintentionally coupling levels |1\rangle and |3\rangle. With this in mind, we assume that the Rabi frequency \( \Omega_{13}(t) \) differs from \( \Omega _{12}(t) \) by a constant complex number, i.e.
\[ \Omega_{13}(t) = \beta e^{i\zeta} \Omega_{12}(t) \] 
(17)
where \( \zeta, \beta \) are real unknown constants, \( \beta \ll 1 \). \( \Omega _{12}(t) \) is the Rabi frequency coupling levels |1\rangle and |2\rangle.

A possible motivation for these assumptions in a quantum-optics setting might be the following: assume that one needs right circularly polarized light (\( \sigma^+ \)) in order to couple states |1\rangle and |2\rangle and one needs left circularly polarized light (\( \sigma^- \)) to couple states |1\rangle and |3\rangle. If the laser light is—instead of exactly right polarized—elliptically polarized, this would cause unwanted transitions to level |3\rangle. Other motivations for these assumptions are possible, especially in other quantum systems (different from the quantum-optics setting of an atom and a classical laser). Note, that these assumptions are also used in [19] with the only difference that in that paper a controllable, time-dependent phase \( \zeta \) has been assumed.

The three levels or bare states of our atom have the following state representation:
\[ |1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} , \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} , \quad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} . \] 
(18)
Hence our Hamiltonian for the three-level system is
\[ H(t) = \frac{\hbar}{2} \begin{pmatrix} -\delta_2(t) \Omega_{12}(t) & \Omega_{12}^*(t) & \beta e^{-i\zeta} \Omega_{13}^*(t) \\ \Omega_{12}(t) & \delta_2(t) & 0 \\ \beta e^{i\zeta} \Omega_{13}(t) & 0 & -2\Delta + \delta_2(t) \end{pmatrix} \] 
(19)
where \( \Delta = \omega_2 - \omega_3 \) is the frequency difference between level |2\rangle and |3\rangle. The phase \( \zeta \) can be absorbed in a redefinition of the basis state for the third level and therefore in the following we will just set \( \zeta = 0 \). We also assume that \( \delta_2(t) = \Omega_{12}(t) = 0 \) for \( t < 0 \) and \( t > T \).

Using the formalism presented in section 2, we can construct schemes which result in full population inversion in the case of no unwanted transition. There is a lot of freedom in choosing the ancillary functions. The goal will be to find the schemes which are very robust against unwanted transitions, i.e. schemes which result in a nearly perfect population inversion even in the presence of an unwanted transition.

3.2. Transition sensitivity
We can write solutions of the time-dependent Schrödinger equation for the Hamiltonian in (19) if \( \beta = 0 \) as follows
\[ |\psi_0(t)\rangle = \begin{pmatrix} \cos (\theta/2) e^{-i\omega_2 t}/2 \\ \sin (\theta/2) e^{-i\omega_2 t}/2 \\ 0 \end{pmatrix} e^{-i\theta t}/2 , \] 
\[ |\psi_1(t)\rangle = \begin{pmatrix} \cos (\theta/2) e^{-i\omega_3 t}/2 \\ \sin (\theta/2) e^{-i\omega_3 t}/2 \\ 0 \end{pmatrix} e^{i\theta t}/2 , \] 
\[ |\psi_2(t)\rangle = \begin{pmatrix} 0 \\ 0 \\ e^{-i\omega_3 t} \end{pmatrix} \] 
(20)
where \( \dot{\Gamma} = \frac{1}{2} (-2\Delta + \delta_2) \). These solutions form an orthonormal basis at every time \( t \). The ancillary functions \( \theta, \alpha, \gamma \) must fulfill equations (5), (6) and (12).

This unwanted coupling to the third level can be regarded as a perturbation using the approximation that \( \beta \) is small. We can write our Hamiltonian (19) as
\[ H(t) = H_0(t) + \beta V(t) \] 
(21)
where \( \beta \) is the strength of the perturbation, \( H_0(t) = H(t)|_{\beta = 0} \) and
\[ V(t) = \frac{\hbar}{2} \begin{pmatrix} 0 & 0 & \Omega_{12}^*(t) \\ 0 & 0 & 0 \\ \Omega_{12}(t) & 0 & 0 \end{pmatrix} . \] 
(22)
Using time-dependent perturbation theory we can calculate the probability of being in state |2\rangle at time \( T \) as
\[ P_2 = 1 - \beta^2 d^2 + O(\beta^4) \] 
(23)
where
\[ q = \frac{1}{i\hbar^2} \sum_{k=0}^{2} \left| \int_0^T dt \langle \psi_0(t)|V(t)|\psi_k(t) \rangle \right|^2. \quad (24) \]

If we substitute in the expression for the perturbation (22) then we get
\[ q = 1 \left| \int_0^T dt \cos \left( \frac{\theta}{2} \right) \sin \theta \hat{\gamma} + i \hat{\gamma} \right|^2 \]
\[ = \left| \int_0^T dt \frac{d}{dt} \sin \left( \frac{\theta(t)}{2} \right) e^{iF(t)+i\Delta t} \right|^2 \quad (25) \]

where \( F(t) = \frac{1}{2} \int_0^t ds (1 + \cos \theta(s)) \hat{\gamma}(s) \). The \( q \) quantifies how sensitive a given protocol (determined by the ancillary functions) is concerning the unwanted transition to level \( \Delta \).

Therefore we will call \( q \) transition sensitivity in the following. Our goal will be to determine protocols or schemes which would maximize \( P_2 \) or equivalently minimize \( q \).

### 3.3. General properties of the transition sensitivity

We will begin by examining some general properties of the transition sensitivity \( q \). First, we note that \( q \) is always independent of \( \alpha \). In the case where \( \hat{\gamma} = 0 \) the transition sensitivity is symmetric about \( \Delta \rightarrow -\Delta \).

In the case of \( \Delta = 0 \), the integral in (25) can be easily evaluated by taking into account that \( \theta(T) = \pi \) and \( \theta(0) = 0 \). From this we see that
\[ q = 1 \text{ if } \Delta = 0. \quad (26) \]

This means there is no possibility in the case of \( \Delta = 0 \) to completely reduce the influence of the unwanted transition.

In the following, we will show that even for \( |\Delta| < 1/T \) the transition probability \( q \) cannot be zero. By partial integration, we get
\[ q = |1 - i\Delta M|^2 = 1 + 2\Delta \text{Im}(M) + \Delta^2 |M|^2 \quad (27) \]

where
\[ M = \int_0^T dt \sin \left( \frac{\theta(t)}{2} \right) \]
\[ \times \exp \left( it - T \Delta - \frac{i}{2} \int_0^T ds (1 + \cos \theta(s)) \hat{\gamma}(s) \right). \quad (28) \]

We have \( q \geq (1 + \Delta \text{Im}(M))^2 \) and
\[ |\text{Im}(M)| \leq \int_0^T dt \left| \sin \left( \frac{\theta(t)}{2} \right) \right| \leq T. \quad (29) \]

Let us assume \( |\Delta|T < 1 \) then
\[ q \geq (1 - |\Delta| |\text{Im}(M)|)^2 \geq (1 - |\Delta| \int_0^T dt \left| \sin \left( \frac{\theta(t)}{2} \right) \right|)^2 \]
\[ \geq (1 - |\Delta|T)^2. \quad (30) \]

So we get \( q > 0 \) if \( |\Delta|T < 1 \), i.e. this means that a necessary condition for \( q = 0 \) is \( T > 1/|\Delta| \).

The next question which we will address is whether there could be a scheme (independent of \( \Delta \)) which results in \( q = 0 \) for all \( |\Delta| > 1/T \). For this we would need
\[ H(\Delta) := \int_0^T dt \frac{d}{dt} [G(t)] e^{i\Delta t} \quad (31) \]

for all \( |\Delta| > 1/T \), where \( G(t) = \sin (\theta(t)/2) e^{iF(t)} \). The left-hand side of this equation, \( H(\Delta) \), is simply the Fourier transform of \( h(t) = \chi_{[0,T]}(t) \frac{d}{dt} [G(t)] \) (where \( \chi_{[0,T]}(t) = 1 \) for \( 0 \leq t \leq T \) and zero otherwise). \( h(t) \) has compact support. If (31) would be true then this would mean that the Fourier transform \( \hat{H}(\Delta) \) of the compactly supported function \( h(t) \) also has compact support. This is not possible and therefore there can be no \( (\Delta)-independent \) protocol which results in \( q = 0 \) for all \( |\Delta| > 1/T \). Nevertheless, we will show below that for a fixed \( \Delta \) there are schemes resulting in \( q = 0 \).

It is also important to examine general properties for \( |\Delta| \gg 1/T \). From the previous remark (and the property that a Fourier transform of any function vanishes at infinity) it is immediately clear that we get \( q \rightarrow 0 \) for \( |\Delta| \rightarrow \infty \). Using partial integration we can derive a series expansion of \( q \) in \( 1/\Delta \).

We use
\[ \int_0^T dt \hat{G}(t) e^{i\Delta t} = -\frac{i}{\Delta} \left[ \hat{G}(t) e^{i\Delta t} \right]_0^T + \frac{i}{\Delta} \int_0^T dt \hat{G}(t) e^{i\Delta t} \]
\[ = -\frac{i}{\Delta} \left[ \hat{G}(t) e^{i\Delta t} \right]_0^T + o \left( \frac{1}{\Delta} \right). \quad (32) \]

Hence, in the case where \( |\Delta| \gg 1/T \) the transition sensitivity is
\[ q = \frac{1}{\Delta^2} \frac{\hat{\theta}(0)^2}{4} + \cdots \quad (33) \]
where we have taken into account that \( \theta(0) = 0 \) and \( \theta(T) = \pi \). By repeating partial integration, we get the higher orders in this \( 1/\Delta \) series.

If we demand
\[ \hat{\theta}(0) = \hat{\theta}(T) = \hat{\theta}(0) = 0 \quad (34) \]
then this first term and the next terms in the \( 1/\Delta \) series expansion of the transition sensitivity vanish. The first non-vanishing term is now
\[ q = \frac{1}{\Delta^2} \frac{\hat{\theta}(0)^2}{4} + \cdots \quad (35) \]

### 3.4. Reference case: flat \( \pi \) pulse

As a reference case we will consider a flat \( \pi \) pulse with
\[ \Omega_R = -\frac{\pi}{T} \sin \alpha, \quad \Omega_I = \frac{\pi}{T} \cos \alpha \quad (36) \]
with a constant phase \( \alpha \). This scheme corresponds to \( \theta(t) = \pi t/T \) and \( \gamma(t) = 0 \).

The transition sensitivity can be easily calculated
\[ q = \left| \int_0^T dt \frac{d}{dt} \left[ \sin \left( \frac{\pi t}{2T} \right) \right] e^{i\Delta t} \right|^2 \]
\[ = \pi^2 \left( 4\Delta^2 T^2 - 4i \Delta T \sin (\Delta T) + \pi^2 \right) \]
\[ \left( \pi^2 - 4\Delta^2 T^2 \right)^2. \quad (37) \]
This transition sensitivity \( q \) is plotted in figures 2(a) and (b). It can be seen that \( q = 1 \) for \( \Delta = 0 \) and it goes to zero for large \( |\Delta| \) as is expected. The transition sensitivity for the flat \( \pi \) pulse is never exactly zero.

### 3.5. Other examples of \( \pi \) pulses

Let us examine two other examples of protocols. Suppose \( \gamma(t) = 0, \theta(t) = 2 \arcsin \left( \frac{t}{T} \right) \). Then we get

\[
q = \left( \frac{1 - e^{i \Delta T}}{\Delta T} \right)^2. \tag{38}
\]

In order to achieve \( q = 0 \) one must have \( T = \frac{2 \pi}{\Delta} \). We also set \( \alpha \) constant and then the associated physical quantities for this protocol are

\[
\delta_2(t) = 0, \quad \Omega_{12}(t) = \frac{2i \epsilon^2}{T \sqrt{1 - \frac{t^2}{T^2}}}. \tag{39}
\]

This is a type of \( \pi \) pulse. Unfortunately the Rabi frequency \( \Omega_{12} \) diverges at \( t = T \). To stop divergence we set

\[
\theta(t) = \frac{\pi}{\arcsin(1 - \epsilon)} \arcsin \left( \frac{1 - \epsilon}{T} \right) \tag{40}
\]

where \( 0 < \epsilon \ll 1 \). By setting \( \alpha = -\pi/2 \) the corresponding Rabi frequency is real (i.e. \( \Omega_r(t) = 0 \) and

\[
\Omega_r(t) = \frac{\pi (1 - \epsilon)}{\arcsin(1 - \epsilon) T \sqrt{1 - \frac{t^2}{T^2}}}. \tag{41}
\]

It also follows that \( \delta_2 = 0 \). The corresponding transition sensitivity with \( \epsilon = 0.01 \) is also plotted in figures 2(a) and (b). Note that this scheme converges for \( \epsilon \to 1 \) to a flat \( \pi \) pulse.

We also construct a scheme fulfilling equations (34) which results in a low \( q \) value for large \( |\Delta| \). For this scheme we set

\[
\theta(t) = -\frac{3 \pi t^4}{T^4} + \frac{4 \pi t^3}{T^3} \tag{42}
\]

and \( \gamma = 0 \). The corresponding transition probability can be seen in figures 2(a) and (b). The corresponding Rabi frequencies can be seen in figure 3. The transition sensitivity for this scheme is lower than that of the flat \( \pi \)-pulse for \( \Delta T > 10 \), meaning it is less sensitive to unwanted transitions. If we set \( \alpha = -\pi/2 \) then we get \( \Omega_r(t) = \frac{\pi^2 \epsilon^2 (1 - \epsilon)}{T^3}, \Omega_r = 0 \) and \( \delta_2 = 0 \).

### 3.6. Numerically optimized scheme with \( q = 0 \)

In the following we will present an example of a class of schemes which can be optimized to achieve a zero transition sensitivity for a fixed \( \Delta \). We use the ansatz

\[
\gamma(t) = c_0 \theta(t), \quad \theta(t) = (\pi - c_1) t/T + c_1 t^3 / T^3 \tag{43}
\]

where the parameters \( c_0 \) and \( c_1 \) were numerically calculated in order to minimize \( q \) for a given \( \Delta \). The result is shown in figure 2(a). As it can be seen, we can construct schemes which make \( q \) vanish for \( \Delta |T| \geq 1.5 \).

\( \alpha(t) \) is chosen so that the Rabi frequency is real. The corresponding Rabi frequency \( \Omega_r \) and the detuning \( \delta_2 \) is shown in figure 4 for different values of \( \Delta T \).

Note that we pick the ansatz (43) because it is simple. It is still possible to optimize the ansatz further for example with the goal of minimizing the maximal Rabi frequency. Moreover, the ansatz could be modified so that the Rabi frequency is zero at initial and final times.
3.7. Comparison of the transition probability

In the following we compare the effectiveness of the different schemes. To do this we compare the exact (numerically calculated) transition probability $P_2$ for the different schemes versus $\beta$ for different values of $\Delta$. This can be seen in figure 5. From this we see that the transition sensitivity is a good indicator of a stable scheme. This is however not the only useful quantity to know about a particular scheme. We also consider the area of the pulse $A := \int_0^T dt \sqrt{\Omega_R^2 + \Omega_I^2}$ and its energy $E := \hbar \int_0^T dt (\Omega_R^2 + \Omega_I^2)$. The values for the different schemes are shown in table 1. It can be seen that the numerically optimized schemes require a higher energy than three different variations of a $\pi$ pulse.

For completeness we also include the following sinusoidal adiabatic scheme [24, 25] in our comparison:

$$\Omega_{12}(t) = \Omega_0 \sin \left( \frac{\pi t}{T} \right),$$

$$\delta_2(t) = -\delta_0 \cos \left( \frac{\pi t}{T} \right). \tag{44}$$

We have chosen $\Omega_0$ so that the adiabatic scheme requires the same energy as the numerically optimized scheme. In addition, we have also optimized the $\delta_0$ to maximize the value of $P_2$ for the error-free case $\beta = 0$. The energy is high enough that the adiabatic scheme results in a nearly perfect population inversion in the error-free case. Nevertheless, the numerically optimized scheme is less sensitive to unwanted transitions, i.e. the numerically optimized scheme results in a higher $P_2$ for non-zero $\beta$.

4. Invariant-based shortcuts in three-level systems

In this section, we will review the derivation of invariant-based STA in three-level systems [17] (for an application see for example [23]). We use a different notation than [17] to underline the connection between the two and three-level Hamiltonians in (1) and (45) respectively (see for example [26]). In addition, we will introduce different boundary conditions for the ancillary functions than those used in [17].
We assume our three-level system has a Hamiltonian of the form
\[
H_{3L}(t) = \frac{\hbar}{2} \begin{pmatrix}
0 & \Omega_{12}(t) & 0 \\
\Omega_{12}(t) & 0 & \Omega_{23}(t) \\
0 & \Omega_{23}(t) & 0
\end{pmatrix}
\]
(45)
where \(\Omega_{12}\) and \(\Omega_{23}\) are real. We also assume that \(\Omega_{12}(t) = \Omega_{23}(t) = 0\) for \(t < 0\) and \(t > T\).

This could for example describe a three-level atom with two on resonance lasers (one coupling states [1] and [2] and the other coupling states [2] and [3]). The Lewis–Riesenfeld invariant for this Hamiltonian is
\[
I(t) = \frac{\hbar}{2} \mu \begin{pmatrix}
-\sin \theta \sin \alpha & -i \cos \theta & 0 \\
\cos \theta \cos \alpha & \sin \theta \cos \alpha & 0 \\
i \sin \theta \sin \alpha & \cos \theta \cos \alpha & 0
\end{pmatrix}
\]
(46)
where \(\mu\) is a constant in units of frequency to keep \(I(t)\) in units of energy. The auxiliary functions \(\alpha(t)\) and \(\theta(t)\) satisfy
\[
\dot{\theta} = \frac{1}{2} (\Omega_{12} \cos \alpha - \Omega_{23} \sin \alpha), \quad \dot{\alpha} = -\frac{i}{2} \cot \theta (\Omega_{23} \cos \alpha + \Omega_{12} \sin \alpha).
\]
(47)
Note the similarity with equations (48). This is due to the aforementioned connection between the two- and three-level Hamiltonians. The eigenstates of \(I(t)\) are
\[
|\phi_0(t)\rangle = \begin{pmatrix}
-\sin \theta \cos \alpha \\
-\cos \theta \\
\sin \theta \sin \alpha
\end{pmatrix},
\]
and
\[
|\phi_{\pm}(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix}
\cos \theta \cos \alpha \pm \sin \alpha \\
-i \sin \theta \\
\pm \cos \theta \sin \alpha \pm i \cos \alpha
\end{pmatrix}
\]
(49)
with eigenvalues \(\lambda_0 = 0\) and \(\lambda_{\pm} = \pm 1\) i.e. \(I(t)|\phi_0(t)\rangle = \lambda_0|\phi_0(t)\rangle\) and the label \(n = 0, \pm\). The Lewis–Riesenfeld phases \(\kappa_n(t)\) are \(\kappa_0 = 0\) and
\[
\kappa_{\pm} = \mp \int_0^t \dot{\theta}(u) (i \cos \theta - \frac{1}{2} (\Omega_{12} \sin \alpha + \Omega_{23} \cos \alpha) \sin \theta) \, du.
\]
(50)
A solution of the time-dependent Schrödinger equation with the Hamiltonian (45) is now \(|\Psi(t)\rangle = e^{i\kappa_0 t} e^{i\kappa_+ t} e^{i\kappa_- t}|\phi_0(t)\rangle\). We impose the following boundary conditions on \(\alpha\) and \(\theta\):
\[
\theta(0) = -\frac{\pi}{2}, \quad \theta(T) = \frac{\pi}{2}, \quad \alpha(0) = 0, \quad \alpha(T) = \frac{\pi}{2}.
\]
(51)
One could impose the following additional boundary conditions in order to make the Rabi frequencies have a finite limit at the initial and final times
\[
\dot{\alpha}(0) = 0, \quad \dot{\alpha}(T) = 0, \quad \dot{\theta}(0) \neq 0, \quad \dot{\theta}(T) \neq 0.
\]
(52)
Note that the boundary conditions given by equations (51) and (52) are an alternative choice to the ones imposed in [17].

Using equations (47) and (48) we can calculate the Rabi frequencies
\[
\Omega_{12}(t) = 2(-\dot{\alpha} \tan \theta \sin \alpha + \dot{\theta} \cos \alpha),
\]
(53)
\[
\Omega_{23}(t) = 2(-\dot{\alpha} \tan \theta \cos \alpha + \dot{\theta} \sin \alpha).
\]
(54)
If the functions \(\alpha\) and \(\theta\) fulfil equations (51) and (52), then the corresponding Rabi frequencies will lead to full population inversion \(|1\rangle \rightarrow |3\rangle\).

### 5. Unwanted transitions in three-level systems

#### 5.1. Model

Now we assume that there is an unwanted coupling to a fourth level as shown in figure 1(c). Analogous to section 3, we assume that the laser coupling levels [2] and [3] also unintentionally couples levels [2] and [4] as well. Hence we assume for the Rabi frequency
\[
\Omega_{24}(t) = \beta e^{i\nu t} \Omega_{23}(t)
\]
(55)
where \(\beta, \nu \in \mathbb{R}\) are unknown constants and \(\beta \ll 1\). The Hamiltonian for this four-level system is given by
\[
H(t) = \frac{\hbar}{2} \begin{pmatrix}
0 & \Omega_{12} & 0 & 0 \\
\Omega_{12} & 0 & \Omega_{23} & \beta e^{-i\nu t} \Omega_{23} \\
0 & \Omega_{23} & 0 & 0 \\
0 & \beta e^{i\nu t} \Omega_{23} & 0 & -2\Delta
\end{pmatrix}
\]
(56)
where \(\Delta = \omega_3 - \omega_4\) and \(h\omega_{ij}\) is the energy of state \(|j\rangle\). As in the previous case, one can redefine the state \(|4\rangle\) to remove the phase. Hence we set \(\nu = 0\) in the following.

Using the formalism presented in section 4, we can construct schemes which result in full population inversion in the case of no unwanted transitions. Again, there is a lot of freedom in choosing the ancillary functions and the goal will be to find the schemes which are stable concerning these unwanted transitions.

#### 5.2. Transition sensitivity

We once again regard this unwanted transition as a perturbation. To treat it as such we write the Hamiltonian as
\[
H(t) = H_0(t) + \beta V(t)
\]
(57)
where \(H_0(t) = H(t)|_{\beta=0}\) and
\[
V(t) = \frac{\hbar}{2} \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & \Omega_{23} \\
0 & \Omega_{23} & 0 & 0
\end{pmatrix}.
\]
(58)
If \(\beta = 0\) then the time-dependent Schrödinger equation for \(H(t)\) has the following set of orthonormal solutions:
\[
|\psi_0(t)\rangle = \begin{pmatrix}
-\sin \theta \cos \alpha \\
-i \cos \theta \sin \alpha \\
0
\end{pmatrix} e^{i\omega_0 t},
\]
\[
|\psi_1(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix}
\cos \theta \cos \alpha + i \sin \alpha \\
-i \sin \theta \\
\cos \theta \sin \alpha + i \cos \alpha
\end{pmatrix} e^{i\omega_+ t},
\]
\[
|\psi_2(t)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix}
\cos \theta \cos \alpha - i \sin \alpha \\
-i \sin \theta \\
\cos \theta \sin \alpha - i \cos \alpha
\end{pmatrix} e^{i\omega_- t},
\]
\[
|\psi_3(t)\rangle = \begin{pmatrix}
0 \\
0 \\
e^{i\Delta t}
\end{pmatrix}.
\]
(59)
Using time-dependent perturbation theory similar to section 3.2, we get for the probability \( P_3 \) to end in the state \( |3\rangle \) at time \( t = T \) that
\[
P_3 = 1 - \beta^2 Q + O (\beta^4).
\]
(60)

where
\[
Q = \int_0^T dt \, e^{i \Delta t} (\dot{\alpha} \sin \theta \cos \alpha + \dot{\theta} \cos \theta \sin \alpha)^2
\]
\[
= \int_0^T dt \, e^{i \Delta t} \frac{d}{dt} (\sin \theta \sin \alpha)^2.
\]
(61)

Similar to section 3, the \( Q \) quantifies how sensitive a given protocol is concerning the unwanted transition to level \( |4\rangle \). As before we will call \( Q \) transition sensitivity in the following and our goal will be to determine protocols or schemes which would minimize \( Q \).

5.3. General properties of the transition sensitivity

We start by examining some general properties of the transition sensitivity \( Q \) given by (61) by noting that \( Q \) is independent of the sign of \( \Delta \). By taking into account the boundary conditions for \( \theta (t) \) and \( \alpha (t) \) we find that
\[
Q = 1 \text{ if } \Delta = 0.
\]
(62)

Similar to section 3.3, we get by partial integration
\[
Q = |1 - i \Delta N|^2 = 1 + 2 \Delta \text{Im} N + \Delta^2 |N|^2
\]
(63)

where
\[
N = -\int_0^T dt \, e^{i \Delta (t-T)} \sin \theta \sin \alpha.
\]
(64)

Therefore \( Q \geq (1 + \Delta \text{Im} (N))^2 \) and
\[
|\text{Im} (N)| \leq \left| \int_0^T dt \, \sin (\Delta (t-T)) \sin \theta \sin \alpha \right|
\]
\[
\leq \int_0^T dt \, |\sin (\Delta (t-T)) | \sin \theta \sin \alpha | \leq T.
\]
(65)

Let us assume \( |\Delta|/T < 1 \) then as before we get
\[
Q \geq (1 - |\Delta| \text{Im} (N))^2 \geq (1 - |\Delta|/T)^2.
\]
(66)

So \( Q > 0 \) if \( |\Delta|/T < 1 \), i.e. a necessary condition for \( Q = 0 \) is \( T > \frac{1}{|\Delta|} \).

Using similar arguments to the ones in section 3.3, we see that in this case as well there can be no \( \Delta \)-independent scheme with \( Q = 0 \) for all \( |\Delta| > 1/T \). Moreover, an approximation of \( Q \) in the case of \( |\Delta|/T > 1 \) can be derived in a similar way as in the previously mentioned section. So we get for \( |\Delta|/T \gg 1 \) that
\[
Q = \frac{1}{\Delta^2} \bar{Q} (0)^2 + \cdots
\]
(67)

taking into account the boundary conditions.

5.4. Example of schemes

As a reference case we consider one of the protocols given in [17]. In this protocol, the following ancillary functions are used
\[
\theta (t) = \epsilon - \frac{\pi}{2}, \quad \alpha (t) = \frac{\pi t}{2T}
\]
(68)

where \( 0 < \epsilon \ll 1 \) and the only difference in boundary conditions being that now \( \theta (T) = -\frac{\pi}{2} \). It should be noted that this protocol does not have perfect population transfer since the boundary conditions are not exactly fulfilled for a non-zero \( \epsilon \). In [17] \( \epsilon = 0.002 \) was deemed sufficient. This protocol has the following Rabi frequencies:
\[
\Omega_{12} (t) = \frac{\pi}{T} \cot \epsilon \sin \left( \frac{\pi t}{2T} \right),
\]
\[
\Omega_{23} (t) = \frac{\pi}{T} \cot \epsilon \cos \left( \frac{\pi t}{2T} \right).
\]
(69)

The transition sensitivity for this scheme is shown in figure 6. Here we note that the derivation of the transition sensitivity is based on exact population transfer in the error free case. Hence it is not strictly correct to consider the transition sensitivity for this protocol. However for the purposes of comparison we include it.

In the following we provide two examples of numerically optimized schemes leading to zero transition sensitivity for some range of \( \Delta \). For the first scheme we use the ansatz
\[
\theta (t) = -\frac{\pi}{2} + (\pi - c_0 - c_1) \frac{t}{T} + c_0 \left( \frac{t}{T} \right)^2 + c_1 \left( \frac{t}{T} \right)^3,
\]
\[
\alpha (t) = \frac{\pi}{4} \sin (\theta (t)) + \frac{\pi}{4}
\]
(70)

where the parameters \( c_0 \) and \( c_1 \) were numerically calculated in order to minimize \( Q \) for a given \( \Delta \). Note that this ansatz automatically avoids any divergences of the corresponding physical potentials for \( 0 \leq t \leq T \). The resulting transition sensitivity \( Q \) is shown in figure 6. As it can be seen, we can construct schemes which make \( Q \) vanish for \( |\Delta|/T \gg 2.5 \). The corresponding Rabi frequencies \( \Omega_{12} \) and \( \Omega_{23} \) are shown in figure 7 for different values of \( \Delta T \).

Another example of a scheme is the following
\[
\theta (t) = -\frac{\pi}{2} - \frac{8(\pi - 2d_0)t^4}{T^4} + 2I(-16d_0 + T + 7\pi) - \frac{I^2(-16d_0 + 3T + 5\pi)}{T^2} + t,
\]

\[
\Delta T
\]

Figure 6. Transition sensitivity \( Q \) versus \( \Delta T \) for different schemes; reference example (\( \epsilon = 0.002 \)) from [17] (blue, thin, dotted line); numerical scheme 1 given by (70) (red, thick, dot-dashed line); numerical scheme 2 given by (71) (green, solid line); lower bound for \( Q \) as in (66) (black, dashed line).
Figure 7. Rabi frequencies for the numerically optimized scheme 1 in (70) versus time $t$; (a) Rabi frequency $\Omega_{12}$; (b) Rabi frequency $\Omega_{23}$; $\Delta T = 0.2$ (red, thick, solid line), $\Delta T = 1.0$ (green, dashed line), $\Delta T = 2.0$ (blue, thin, solid line), $\Delta T = 3.0$ (black, dotted line).

Figure 8. Rabi frequencies for the numerically optimized scheme 2 in (71) versus time $t$; (a) Rabi frequency $\Omega_{12}$; (b) Rabi frequency $\Omega_{23}$; $\Delta T = 0.2$ (red, thick, solid line), $\Delta T = 1.0$ (green, dashed line), $\Delta T = 2.0$ (blue, thin, solid line), $\Delta T = 3.0$ (black, dotted line).

Figure 9. Transition probability $P_3$ versus perturbation strength $\beta$ for different schemes: reference example ($\epsilon = 0.002$) from [17] (red, thick, solid line); numerical scheme 1 given by (70) (black, dotted line); numerical scheme 2 given by (71) (blue, thin, solid line); adiabatic scheme (green, thick, dashed line); (a) $\Delta T = 1.0$, (b) $\Delta T = 3.0$.

We compare the scheme of the schemes proposed in [17] as a reference scheme, the numerical scheme 1 given by (70) and the numerical scheme 2 given by (71). Once again we see that the transition sensitivity is a good indicator of a stable scheme. We also consider the area of the pulse and its energy which in this case is defined as $A := \frac{\pi}{T} \left( \int_0^T dt \sqrt{\Omega_{12}^2 + \Omega_{23}^2} \right)$ respectively. These values are shown for each scheme in table 2.

For completeness we also include the following adiabatic STIRAP-like scheme in our comparison [27]:

\begin{align}
\Omega_{12} &= \Omega_0 \sin \left( \frac{\pi t}{2T} \right), \\
\Omega_{23} &= \Omega_0 \cos \left( \frac{\pi t}{2T} \right).
\end{align}

$\Omega_0$ was chosen so that the adiabatic scheme has the same energy as the numerical scheme 1.
Both numerically-optimized schemes result in the largest $P_3$ in figure 9(a) if $\beta \neq 0$ for $\Delta T = 1.0$. If $\Delta T = 3.0$, see figure 9(b), then both numerical-optimized schemes result in nearly full population transfer even in the case of $-0.1 < \beta < 0.1$. It can be seen that a full population transfer is not achieved in both cases by this adiabatic scheme for $\beta = 0$.

6. Conclusion

In this paper, we have developed STA schemes in two- and three-level quantum systems which lead to nearly perfect population inversion even in the presence of an additional unwanted and uncontrollable transition. For the two-level case as well as for the three-level case, this has been based on the definition of a transition sensitivity which quantifies how sensitive a given scheme is concerning these unwanted couplings to another level. We have provided examples of shortcut schemes leading to a zero transition sensitivity (and hence almost full population transfer) in certain regimes.

The developed shortcut schemes can easily be adapted to other quantum settings. Additionally, the proposed schemes may be simpler to implement experimentally than previous methods which require a control of the phase of the unwanted transition. Hence, the results of this paper could be important in quantum information processing or other applications which require fast quantum control with high fidelity.

The approach of this paper could be even further generalized; one could construct different shortcut schemes fulfilling even further constraints apart from vanishing transition sensitivity similar to [15]. This work could also be generalized to different level structures of the unwanted transitions or to multiple unwanted transition channels. In the latter case, one might expect to find that the unwanted transition with lowest detuning would dominate.