Optimally robust shortcuts to population inversion in two-level quantum systems

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Abstract. We examine the stability versus different types of perturbations of recently proposed shortcuts to adiabaticity to speed up the population inversion of a two-level quantum system. We find the optimally robust processes by using invariant-based engineering of the Hamiltonian. Amplitude noise and systematic errors require different optimal protocols.

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## 1. Introduction

Manipulating the state of a quantum system with time-dependent interacting fields is a fundamental operation in atomic and molecular physics, with applications such as laser-controlled chemical reactions, metrology, interferometry, nuclear magnetic resonance or quantum information processing [1–5]. For two-level systems, there are several approaches proposed for attaining a complete population transfer, for example, $\pi$ pulses, composite pulses, adiabatic passage and its variants. In general, the $\pi$ pulses may be fast but highly sensitive to variations in the pulse area, and to inhomogeneities in the sample [1]. Used first in nuclear magnetic resonance [6], composite pulses provide an alternative to the single $\pi$ pulse, with some successful applications [7, 8], but still need accurate control of pulse phase and intensity. A robust option is, in principle, adiabatic (slow) passage, which is however prone to decoherence because of the effect of noise over the long times required. A compromise is to use speeded-up ‘shortcuts to adiabaticity’, which may be broadly defined as the processes that lead to the same final populations as the adiabatic approach in a shorter time.

Several methods to find shortcuts to adiabaticity have been put forward [9–19] for two- and three-level atomic systems. The transitionless or counter-diabatic (CD) control protocols proposed by Demirplak and Rice [9] and Berry [10] start from a reference time-dependent Hamiltonian $H_0$ and provide an extra interaction that cancels the diabatic couplings. This results in an exact following of the adiabatic dynamics of the reference Hamiltonian, in principle in an arbitrarily short time. They have been applied, for example, to speed up the rapid adiabatic passage (RAP) for an Allen–Eberly scheme [11]. Modified by a unitary transformation [17],

## Contents

1. Introduction 2
2. Shortcuts to adiabatic passage for a two-level quantum system 3
   2.1. A $\pi$ pulse 4
   2.2. Adiabatic schemes and transitionless shortcuts to adiabaticity 4
   2.3. Inverse engineering of invariant-based shortcuts 5
3. General formalism for systematic and amplitude-noise errors 6
4. Amplitude-noise errors 7
   4.1. Example: $\pi$ pulse with a real Rabi frequency 8
   4.2. Example of a transitionless protocol 9
   4.3. Optimal scheme 10
5. Systematic errors 12
   5.1. Example: $\pi$ pulse 12
   5.2. Example of a transitionless shortcut 13
   5.3. Optimal scheme 13
6. Systematic and amplitude-noise errors 15
Acknowledgments 17
Appendix. Derivation of the master equation for amplitude-noise error 17
References 18
the transitionless quantum driving has been experimentally implemented for a two-level system realized by Bose–Einstein condensates in optical lattices [16].

Another shortcut technique is to inverse engineer the Hamiltonian using the Lewis–Riesenfeld invariants [20], as in [21–33]. The invariant-based method has been applied to accelerate the adiabatic processes for trap expansion or compressions [21–27] and atomic transport [28–30]. It has also been combined with optimal control theory [24, 30], and proposed for other applications [17, 31–33]. CD and invariant-based engineering can, in fact, be shown to be potentially equivalent methods by properly adjusting the reference Hamiltonian [14]. In standard applications however, $H_0$ is set according to some predetermined protocol (for example, the Landau–Zener, Allen–Eberly or finite-time schemes), and the formulation and results of the two methods are generally quite different, so they may be considered, in practice, separate approaches.

A key element to choose among the fast protocols is their stability or robustness versus different perturbations. In many experiments, the main source of error is the deviations in the coupling term: for example, due to fluctuations in the laser intensity in an atom–laser realization of the two-level system, or an inaccurate realization of the ideal function. In this work, we examine the stability with respect to the amplitude noise of the interaction and with respect to systematic errors. We will compare the results with ordinary (flat) $\pi$ pulses and explore the stability of the transitionless approach with respect to parameter variations for a finite-time sinusoidal protocol for $H_0$.

The main aim of this paper is to find optimal protocols with respect to these error sources. The optimality will be determined by minimizing properly defined sensitivities. It turns out that the perturbations due to noise and systematic errors require different optimal protocols, and we shall use invariant-based inverse engineering to find them.

The rest of the paper is organized as follows. In section 2, we shall review the transitionless-based shortcuts protocol and the invariant-based one. In section 3, the general formalism to model amplitude-noise error and systematic error will be presented. The special case of solely amplitude-noise error will be examined in section 4 where the noise sensitivity of the different protocols will be studied and the most stable protocol will be derived. In section 5, the special case of solely systematic error will be studied and the most stable protocol will be derived. The general case of amplitude noise as well as systematic noise for the different protocols will be numerically studied in section 6.

2. Shortcuts to adiabatic passage for a two-level quantum system

We assume a two-level system with a Hamiltonian of the form

$$H_0(t) = \frac{\hbar}{2} \begin{pmatrix} \Omega_R(t) - \Delta(t) & \Omega_I(t) - i \Omega_1(t) \\ -\Omega_I(t) + i \Omega_1(t) & \Omega_R(t) - \Delta(t) \end{pmatrix}.$$  (1)

For example, in quantum optics such a Hamiltonian describes the semiclassical coupling of two atomic levels with a laser in a laser-adapted interaction picture. In that setting $\Omega(t) = \Omega_R(t) + i \Omega_I(t)$ would be the complex Rabi frequency (where $\Omega_R$ and $\Omega_I$ are the real and imaginary parts) and $\Delta$ would be the time-dependent detuning between laser and transition frequencies. We find it convenient to keep the language of the atom–laser interaction hereafter, noting that in other two-level systems $\Omega(t)$ and $\Delta(t)$ will correspond to different physical quantities and that
instead of ‘atom’ one may refer, for example, to a spin-1/2 or to a Bose–Einstein condensate on an accelerated optical lattice [16].

Initially, at time $t = 0$, the atom is in the ground state $|1\rangle = \left(\frac{1}{\sqrt{2}} \right)$. Often the goal is to achieve a perfect population inversion such that at a time $t = T$ the atom is in the excited state $|2\rangle = \left(\frac{1}{\sqrt{2}} \right)$. The time $T$ should be as small as possible, but also the scheme or protocol to achieve this population inversion should be as stable as possible concerning errors. In the following subsections, we will review different schemes to achieve a population inversion before we discuss different types of possible error sources in the next section.

2.1. A $\pi$ pulse

A simple scheme to achieve population inversion is a $\pi$ pulse. In this case the laser is in resonance, i.e. the detuning is zero $\Delta(t) = 0$ for all $t$. If the Rabi frequency is chosen as $\Omega(t) = |\Omega(t)| e^{i\omega t}$, with a time-independent $\alpha$, and such that

$$\int_0^T dt \ |\Omega(t)| = \pi,$$

(2)

the population is inverted at time $T$. A simple example is the ‘flat’ $\pi$ pulse with $\Omega(t) = \frac{\pi}{T} e^{i\omega}$. 

2.2. Adiabatic schemes and transitionless shortcuts to adiabaticity

The population inversion may also be achieved by an adiabatic scheme. Let the instantaneous eigenstates of the Hamiltonian $H_0$ be $|n(t)\rangle$. The adiabatic theorem tells us that if we start in an eigenstate at $t = 0$, i.e. $|\psi(0)\rangle = |n(0)\rangle$, and if we vary the Hamiltonian infinitesimally slowly, then the system will stay in the corresponding instantaneous eigenstate for all times, up to a phase factor, i.e. $|\psi(t)\rangle \approx e^{i\lambda_n(t)}|n(t)\rangle$. If the eigenstate corresponds initially to the ground state $|1\rangle$ and at $t = T$ to the excited state $|2\rangle$ (up to a phase), then we would achieve a perfect population inversion as $T \rightarrow \infty$.

Demirplak and Rice [9] and independently Berry [10] proposed a modification of the Hamiltonian such that the state would exactly follow the instantaneous eigenstate of the Hamiltonian $H_0$ for an arbitrary duration $T$. If the desired time-evolution operator is $U = \sum e^{i\lambda_n(t)}|n(t)\rangle \langle n(0)|$, the corresponding Hamiltonian leading to this time evolution is $H_{0a}(t) = i\hbar \left( \frac{\partial}{\partial t} U \right) U^\dagger$. We may write $H_{0a} = H_0 + H_a$, where $H_a = i\hbar \sum_n |\partial_t n(t)\rangle \langle n(t)|$ is the ‘counter-diabatic’ term that guarantees that the system will follow the instantaneous eigenstates of $H_0$ without transitions even for a small $T$. This method is thus termed the counter-diabatic approach or transitionless-tracking algorithm.

For the two-level system with Hamiltonian $H_0$ and $\Omega_1 = 0$, the additional Hamiltonian takes the form

$$H_a(t) = \frac{\hbar}{2} \begin{pmatrix} 0 & -i\Omega_a(t) \\ i\Omega_a(t) & 0 \end{pmatrix},$$

(3)

with $\Omega_a \equiv [\Omega_R \dot{\Delta} - \dot{\Omega}_R \Delta]/(\Delta^2 + \Omega_R^2)$. The total Hamiltonian is therefore [11]

$$H_{0a}(t) = \frac{\hbar}{2} \begin{pmatrix} -\Delta & \Omega_R - i\Omega_a \\ \Omega_R + i\Omega_a & \Delta \end{pmatrix},$$

(4)

which sets the transitionless shortcut protocol. With this protocol, population inversion is always achieved even if the adiabatic condition fails for $H_0$.
2.3. Inverse engineering of invariant-based shortcuts

Shortcuts to adiabaticity can also be found by making explicit use of the Lewis–Riesenfeld invariants. For the general Hamiltonian $H_0$ in (1), a dynamical invariant of the corresponding Schrödinger equation (this is a Hermitian operator $I(t)$ fulfilling $\frac{d}{dt} I + \frac{i}{\hbar} [H_0, I] = 0$, so that its expectation values remain constant) is given by

$$I(t) = \frac{\hbar}{2\mu} \begin{pmatrix} \cos (\Theta(t)) & e^{-i\alpha(t)} \sin (\Theta(t)) \\ e^{i\alpha(t)} \sin (\Theta(t)) & -\cos (\Theta(t)) \end{pmatrix},$$

where $\mu$ is an arbitrary constant with units of frequency to keep $I(t)$ with dimensions of energy, and the functions $\Theta(t)$ and $\alpha(t)$ satisfy the differential equations

$$\dot{\Theta} = \Omega_I \cos \alpha - \Omega_R \sin \alpha,$$

$$\dot{\alpha} = -\Delta - \cot \Theta (\cos \alpha \Omega_R + \sin \alpha \Omega_I).$$

The eigenvectors of the invariant are

$$|\phi_+(t)\rangle = \begin{pmatrix} \cos (\Theta/2) e^{-i\alpha/2} \\ \sin (\Theta/2) e^{i\alpha/2} \end{pmatrix}, \quad |\phi_-(t)\rangle = \begin{pmatrix} \sin (\Theta/2) e^{-i\alpha/2} \\ -\cos (\Theta/2) e^{i\alpha/2} \end{pmatrix},$$

with the eigenvalues $\pm \frac{\hbar}{2} \mu$. A general solution $|\Psi(t)\rangle$ of the Schrödinger equation can be written as a linear combination $|\Psi(t)\rangle = c_+ e^{i\kappa_+ t} |\phi_+(t)\rangle + c_- e^{i\kappa_- t} |\phi_-(t)\rangle$, where $c_\pm$ are complex, constant coefficients and $\kappa_\pm$ are the Lewis–Riesenfeld phases [20]

$$\dot{\kappa}_+ = \frac{1}{\hbar} \langle \phi_+ | i \hbar \frac{\partial}{\partial t} - H_0 | \phi_+ \rangle,$$

$$\dot{\kappa}_- = \frac{1}{\hbar} \langle \phi_- | i \hbar \frac{\partial}{\partial t} - H_0 | \phi_- \rangle.$$

In particular, we may construct the solution

$$|\psi(t)\rangle = |\phi_+(t)\rangle e^{-i\gamma(t)/2} = \begin{pmatrix} \cos(\Theta/2)e^{-i\alpha/2} \\ \sin(\Theta/2)e^{i\alpha/2} \end{pmatrix} e^{-i\gamma/2}$$

and the orthogonal solution (for all times $\langle \psi_\perp | \psi \rangle = 0$)

$$|\psi_\perp(t)\rangle = |\phi_-(t)\rangle e^{i\gamma(t)/2} = \begin{pmatrix} \sin(\Theta/2)e^{-i\alpha/2} \\ -\cos(\Theta/2)e^{i\alpha/2} \end{pmatrix} e^{i\gamma/2},$$

where

$$\gamma = -2\kappa_+ = 2\kappa_-.$$

Finally, we obtain

$$\dot{\gamma} = \frac{1}{\sin \Theta} (\cos \alpha \Omega_R + \sin \alpha \Omega_I).$$

Equivalently, we may design a solution of the Schrödinger equation $|\psi(t)\rangle$ with the parameterization of a pure state given in (8). (Note that $|\psi(t)\rangle\langle \psi(t) |$ is a dynamical invariant.) By putting this ansatz into the Schrödinger equation, we obtain immediately (6) and (10). A solution that is orthogonal to (8), i.e. $\langle \psi_\perp | \psi \rangle = 0$ for all times, is then directly given by (9).
The next step to find invariant-based shortcuts is to inverse engineer the Hamiltonian. For achieving a population inversion, the boundary values should be \( \Theta(0) = 0 \) and \( \Theta(T) = \pi \), so
\[
|\psi(0)\rangle = \left( e^{-i\alpha(0)/2} \right) e^{-i\gamma(0)/2}, \quad |\psi(T)\rangle = \left( 0 \right) e^{-i\gamma(T)/2}.
\]
Assume that \( \Theta(t), \alpha(t) \) and \( \gamma(t) \) are given, with \( \Theta(0) = 0 \) and \( \Theta(T) = \pi \). Then we obtain the Hamiltonian corresponding to solution (8) by inverting (6) and (10). This leads to
\[
\Omega_R = \cos \alpha \sin \dot{\Theta} - \sin \alpha \dot{\Theta}, \quad (11)
\]
\[
\Omega_i = \sin \alpha \sin \dot{\Theta} + \cos \alpha \dot{\Theta}, \quad (12)
\]
\[
\Delta = - \cos \Theta \dot{\gamma} - \dot{\alpha}. \quad (13)
\]
By implementing these functions exactly, the population would be inverted in the unperturbed, error-free case. Note that invariant-based shortcuts and transitionless shortcuts may be formally related, see [14].

3. General formalism for systematic and amplitude-noise errors

We shall now consider systematic errors as well as noise-related errors. Let the ideal, unperturbed Hamiltonian be \( H_0 \). For systematic errors, the actual, experimentally implemented Hamiltonian is \( H_{01} = H_0 + \beta H_1 \), but the evolution of the pure quantum state is still described by the Schrödinger equation with the perturbed Hamiltonian \( H_{01} \). Sometimes systematic errors cannot be avoided, for example if atoms at different positions are subjected to slightly different fields, due to the Gaussian shape of the laser inducing different Rabi frequencies. It is thus desirable to have protocols that are very stable with respect to perturbed Hamiltonian functions.

The second type of error is a stochastic one, i.e. the Hamiltonian \( H_{01} \) is perturbed by some stochastic part \( \lambda H_2 \) describing amplitude noise. A stochastic Schrödinger equation (in the Stratonovich sense) is then
\[
i \hbar \frac{d}{dt} \psi(t) = (H_{01} + \lambda H_2 \xi(t)) \psi(t),
\]
where \( \xi(t) = \frac{dw}{dt} \) is heuristically the time derivative of the Brownian motion \( W_t \). We have \( \langle \xi(t) \rangle = 0 \) and \( \langle \xi(t) \xi(t') \rangle = \delta(t - t') \) because the noise should have zero mean and the noise at different times should be uncorrelated. If we average over different realizations and define \( \rho(t) = \langle \rho_{\xi} \rangle \), then \( \rho(t) \) satisfies
\[
\frac{d}{dt} \rho = -i \frac{\hbar}{\lambda} [H_{01}, \rho] - \frac{\lambda^2}{2\hbar^2} [H_2, [H_2, \rho]]. \quad (14)
\]
Further details of the derivation can be found in the appendix.

We may consider the two effects together with the master equation
\[
\frac{d}{dt} \rho = -i \frac{\hbar}{\lambda} [H_0 + \beta H_1, \rho] - \frac{\lambda^2}{2\hbar^2} [H_2, [H_2, \rho]], \quad (15)
\]
where \( \beta \) is the amplitude of the systematic noise described by the Hamiltonian \( H_1 \) and \( \lambda \) is the strength of the amplitude noise.
In this paper, we assume that the errors affect the frequencies $\Omega_R$ and $\Omega_I$ but not the detuning $\Delta$, which, for an atom–laser realization of the two-level system, is more easily controlled. For the systematic error we restrict ourselves to an error Hamiltonian of the form

$$H_1(t) = \frac{\hbar}{2} \begin{pmatrix} \Omega_R(t) & -i\Omega_I(t) \\ i\Omega_I(t) & \Omega_R(t) \end{pmatrix} = H_0(t) \bigg|_{\Delta=0},$$

(16)

For the noise error we restrict ourselves to independent amplitude noise in $\Omega_R$ as well as in $\Omega_I$ with the same intensity $\lambda^2$, i.e. the final master equation is

$$\frac{d}{dt} \rho = -\frac{i}{\hbar} [H_0 + \beta H_1, \rho] - \frac{\lambda^2}{2\hbar^2} \left( [H_2R, [H_2R, \rho]] + [H_{2I}, [H_{2I}, \rho]] \right),$$

(17)

where

$$H_{2R}(t) = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega_R(t) \\ \Omega_R(t) & 0 \end{pmatrix}, \quad H_{2I}(t) = \frac{\hbar}{2} \begin{pmatrix} 0 & -i\Omega_I(t) \\ i\Omega_I(t) & 0 \end{pmatrix}.$$

A motivation for this modeling is that two different lasers may be used to implement the two parts of the Rabi frequency.

It is now convenient to represent the density matrix $\rho(t)$ by the Bloch vector

$$\vec{r}(t) = \begin{pmatrix} \rho_{12} + \rho_{21} \\ i(\rho_{12} - \rho_{21}) \\ \rho_{11} - \rho_{22} \end{pmatrix} ,$$

such that $\rho = \frac{1}{2}(1 + \vec{r} \cdot \vec{\sigma})$ where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices. The Bloch equation corresponding to the master equation (17) is

$$\frac{d}{dt} \vec{r} = (\hat{L}_0 + \beta \hat{L}_1 - \lambda^2 \hat{L}_2)\vec{r},$$

(18)

where

$$\hat{L}_0 = \begin{pmatrix} 0 & \Delta(t) & \Omega_I(t) \\ -\Delta(t) & 0 & -\Omega_R(t) \\ -\Omega_I(t) & \Omega_R(t) & 0 \end{pmatrix}, \quad \hat{L}_1 = \begin{pmatrix} 0 & 0 & \Omega_I(t) \\ 0 & 0 & -\Omega_R(t) \\ -\Omega_I(t) & \Omega_R(t) & 0 \end{pmatrix}$$

and

$$\hat{L}_2 = \frac{1}{2} \begin{pmatrix} \Omega_I(t)^2 & 0 & 0 \\ 0 & \Omega_R(t)^2 & 0 \\ 0 & 0 & \Omega_R(t)^2 + \Omega_I(t)^2 \end{pmatrix}.$$

Note that the probability to be in the excited state at time $t$ is $P_2(t) = \frac{1}{2}(1 - r_3(t))$. In the following section we will first study the amplitude-noise errors only and then in section 5 the systematic errors and finally both together.

4. Amplitude-noise errors

We assume that there is an amplitude-noise type or error affecting the Rabi frequencies and no systematic errors ($\beta = 0$). Let us define the noise sensitivity as

$$q_N := -\frac{1}{2} \frac{\partial^2 P_2}{\partial \lambda^2} \bigg|_{\lambda=0} = -\frac{\partial P_2}{\partial (\lambda^2)} \bigg|_{\lambda=0}.$$

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where $P_2$ is the probability to be in the excited state at the final time $T$, i.e. $P_2 \approx 1 - q_N \lambda^2$. A smaller value of $q_N$ means less sensitivity with respect to amplitude-noise errors, i.e. the scheme is more stable concerning this type of noise. In general, an analytic solution of the master equation (17) or the Bloch equation (18) cannot be found. To calculate $q_N$ we do a perturbation approximation of the solution keeping only terms up to $\lambda^2$ (with $\beta = 0$). In this manner, we obtain

$$r_3(T) = (0, 0, 1)\tilde{r}(T)$$

$$\approx r_{0,3}(T) - \lambda^2 \int_0^T dt' (0, 0, 1)\tilde{U}_0(T, t')\hat{L}_2(t')\tilde{r}_0(t')$$

$$\approx r_{0,3}(T) + \lambda^2 \int_0^T dt' (0, 0, -1)\tilde{U}_0(T, t')\hat{L}_2(t')\tilde{r}_0(t'),$$

where $\tilde{U}_0$ is the unperturbed time-evolution operator for the Bloch vector. If the noiseless scheme works perfectly, i.e. $r_{0,3}(T) = -1$, then

$$P_2 = 1 - \frac{\lambda^2}{2} \int_0^T dt' \tilde{r}_0(t')^T\hat{L}_2(t')\tilde{r}_0(t'),$$

where $^T$ means the transpose operation and the noise sensitivity becomes

$$q_N = \frac{1}{2} \int_0^T dt' \tilde{r}_0(t')^T\hat{L}_2(t')\tilde{r}_0(t)$$

$$= \frac{1}{4} \int_0^T dt [\Omega_1(t)^2(r_{0,1}(t)^2 + r_{0,3}(t)^2) + \Omega_R(t)^2(r_{0,2}(t)^2 + r_{0,3}(t)^2)].$$

(19)

4.1. Example: $\pi$ pulse with a real Rabi frequency

As a first simple example of a population-inversion protocol, we look at a $\pi$ pulse with a real Rabi frequency, i.e. we set $\Delta = 0$, $\Omega_1 = 0$ and $\int_0^T \Omega_R(t) \, dt = \pi$. In this case the master equation, respectively the Bloch equation for amplitude noise, can be solved analytically. The solutions of this equation with the initial conditions $\rho_{11}(0) = 1$, $\rho_{12}(0) = \rho_{21}(0) = \rho_{22}(0) = 0$ respectively $\tilde{r}(0) = (0, 0, 1)^T$ at initial time $t = 0$ are

$$r_1(t) = 0,$$

$$r_2(t) = -e^{-\lambda^2\int_0^t \omega_R^2(t')/2} \sin \left( \int_0^t \Omega_R(t') \, dt' \right),$$

$$r_3(t) = e^{-\lambda^2\int_0^t \omega_R^2(t')/2} \cos \left( \int_0^t \Omega_R(t') \, dt' \right),$$

(20)

which yields

$$P_2 = \frac{1}{2} - \frac{1}{2}r_3(T) = \frac{1}{2} + \frac{1}{2}e^{-\lambda^2\int_0^T \omega_R^2(t)/2}. $$

The noise sensitivity is now

$$q_N = \frac{1}{4} \int_0^T dt \, \Omega_R^2(t),$$

(21)
Figure 1. Probability $P_2$ to end in the excited state at time $T$ versus noise parameter $\lambda$: the minimal noise sensitivity (MNS)-optimal protocol (green, dashed line), flat $\pi$ pulse with purely real Rabi frequency (blue, dotted line), sinusoidal RAP protocol (black, dashed-dotted line) and transitionless shortcut method (red, solid line). Additional parameters for the sinusoidal RAP protocol and the transitionless protocol: $\Omega_0 T = 5.57/4.3 \pi$, $\delta_0 T = (5.57/4.3)^2 \pi$.

which may be bounded as $\frac{\pi^2}{4 T^2} \leq q_N \leq \frac{\pi}{T} \max_{0 \leq t \leq T} |\Omega_R(t)|$, where the lower bound is derived using the Schwartz inequality, i.e. $\int_0^T dt \Omega_R(t)^2 \leq \int_0^T dt \Omega_R^2(t)$. We can achieve the lower bound using a constant $\Omega_R = \pi/T$ (i.e. a flat $\pi$ pulse). The excitation probability $P_2$ for this flat $\pi$ pulse is plotted in figure 1 versus the noise intensity $\lambda$ (blue, dotted line). The noise sensitivity is $q_N = \pi^2/4T \approx 2.467/T$. The other lines in figure 1 correspond to different protocols, see below for more details. The important thing at this point is to note that the stability of a protocol is very well quantified by $q_N$, which is the curvature at $\lambda = 0$.

### 4.2. Example of a transitionless protocol

As another example, we will now look at the stability and noise sensitivity of a transitionless shortcut protocol. Our reference scheme is an adiabatic scheme, see section 2.2, namely the finite-time sinusoidal RAP protocol [34, 35]

$$\Omega_R(t) = \Omega_0 \sin \left( \frac{\pi t}{T} \right), \quad \Delta(t) = -\delta_0 \cos \left( \frac{\pi t}{T} \right),$$

with $\Omega_1 = 0$ and $0 \leq t \leq T$. The excitation probability for this protocol is also shown in figure 1 (black, dashed-dotted line). The chosen parameters $\Omega_0$, $\delta_0$ are not large enough to fulfil the adiabatic condition, so a shortcut to adiabaticity may be used for a full population inversion.

Figure 1 shows the excitation probability also for the transitionless shortcut based on this sinusoidal model (red, solid line). The noise sensitivity of this protocol is $q_N = 3.21/T$. Figure 2 shows the noise sensitivity for the transitionless protocol based on the sinusoidal model (22) for different values of $\delta_0$ and $\Omega_0$. The minimal noise sensitivity (MNS) in this figure is achieved for $\delta_0 = \Omega_0 = 0.5/T$ and has the value $q_N = 2.475/T$, which is very close to the noise sensitivity of the flat $\pi$ pulse in the previous subsection.
4.3. Optimal scheme

We can also write the unperturbed Bloch vector in the form

$$\vec{r}_0(t) = \begin{pmatrix} \sin \Theta \cos \alpha \\ \sin \Theta \sin \alpha \\ \cos \Theta \end{pmatrix}. \quad (23)$$

This Bloch vector corresponds to the pure state in (8). Therefore, we obtain from the Bloch equation the same equations (6). If the trajectory of the Bloch vector $\vec{r}(t)$ and $\gamma(t)$ is given, i.e. $\Theta$, $\alpha$ and $\gamma$ are given, then the corresponding $\Omega_R$ and $\Omega_I$ can be calculated by (11) and (12).

In the following, it is more convenient to use $\Theta(t)$, $\alpha(t)$ and $m(t) = -\dot{\gamma} \sin \Theta$ as independent functions. (Recall that an additive constant in $\gamma$ corresponds to a global phase shift and is therefore irrelevant.) Using (11), (12), (19) and (23), we obtain for the noise error sensitivity

$$q_N = \int_0^T dt \left[ \left( \cos^2 \Theta + \cos^2 \alpha \sin^2 \Theta \right) (m \sin \alpha - \cos \alpha \dot{\Theta})^2 \\
+ \left( \cos^2 \Theta + \sin^2 \alpha \sin^2 \Theta \right) (m \cos \alpha + \sin \alpha \dot{\Theta})^2 \right]$$

$$\equiv \int_0^T dt L(m, \alpha, \Theta, \dot{\Theta}), \quad (24)$$

where $L$ is the Lagrange function for $q_N$. We are looking for functions $m(t)$, $\Theta(t)$, $\alpha(t)$ which minimize this functional. From the Euler–Lagrange formalism, we obtain

$$0 = \frac{\partial L}{\partial m} \Rightarrow m = \frac{\dot{\Theta} \sin(4\alpha) \sin^2 \Theta}{4 \cos^2 \Theta + 2 \sin^2(2\alpha) \sin^2 \Theta}.$$

Moreover,

$$0 = \frac{\partial L}{\partial \alpha} \Rightarrow \sin(4\alpha) = 0 \Rightarrow \alpha = n\pi/4.$$

From this it also follows that $m(t) = 0$. Finally, we have

$$0 = \frac{\partial L}{\partial \Theta} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\Theta}}. \quad (25)$$

Let us now consider the cases of $n$ odd and $n$ even separately.
The case of $n$ even. If $n$ is even, then (25) simplifies to $\dot{\Theta} = 0$. Taking into account the boundary conditions $\Theta(0) = 0, \Theta(T) = \pi$, we arrive at

$$\Theta(t) = \pi t / T.$$  

It follows that

$$\Omega_R = -\sin \left( \frac{n\pi}{4} \right) \frac{\pi}{T}, \quad \Omega_I = \cos \left( \frac{n\pi}{4} \right) \frac{\pi}{T}, \quad \Delta = 0.$$  

Note that either $\Omega_R$ or $\Omega_I$ is zero, so these schemes are flat $\pi$ pulses with a purely real or purely imaginary Rabi frequency. (As an example, we obtain for $n = 6$ a $\pi$ pulse with a flat, real Rabi frequency $\Omega_R = \frac{\pi}{T}$ and $\Omega_I = 0$.) For all these schemes, an analytical solution of the master equation can be derived similar to the one in section 4.1, and the noise sensitivity of all schemes is $q_N = \pi^2 / (4T)$.

The case of $n$ odd. For $n$ odd we obtain

$$\left( 3 + \cos(2\Theta) \right) \dot{\Theta} = \sin(2\Theta)(\dot{\Theta})^2.$$  

Then $\Omega_R = \pm \dot{\Theta} / \sqrt{2} = \pm \Omega_1$ and $\Delta(t) = 0$. In the following, we will call these protocols (for $n$ odd) minimal noise sensitivity (MNS) optimal protocols because we will see below that they are less sensitive to amplitude noise than the $n$ even protocols. Similarly to the previous case, we also obtain now

$$\Delta = 0, \quad \int_0^T dt \sqrt{\Omega_R^2 + \Omega_I^2} = \int_0^T d\dot{\Theta}(t) = \pi,$$

which means that the MNS-optimal protocol is a special case of a $\pi$ pulse. We first solve (26) for $\Theta$ numerically and then put the solution in the expression for the noise sensitivity. The numerically calculated $\Theta(t)$ can be seen in figure 3 (solid line, left axis). The corresponding Rabi frequencies for $n = 7$ are $\Omega_R(t) = \Omega_1(t) = \Omega(t)$, where $\Omega$ is also shown in figure 3 (dashed line, the right axis). Note that for other values of odd $n$, only the signs of $\Omega_R$, respectively $\Omega_I$, are switched. The noise sensitivity value is $q_N = 1.82424 / T < \pi^2 / (4T)$. Therefore, for $n$ odd, smaller noise sensitivities can be achieved than for $n$ even. The excitation probability $P_2$ at time $T$ versus $\lambda$ of the MNS-optimal protocol is also shown in figure 1 (green, dashed line).

**Figure 3.** MNS-optimal protocol: $\Theta(t)$ (blue, solid line; the left axis) and $\Omega(t)$ (red, dashed line; the right axis).
An approximate solution of (26) is given by $\Theta(t) = \pi t / T = \frac{\pi}{\frac{1}{12}} \sin(2\pi t / T)$, with a noise sensitivity of $\eta_n = 1.82538 / T$. The corresponding Rabi frequencies fulfil $|\Omega_r| = |\Omega_i| = \frac{\pi}{6\sqrt{2T}} (6 - \cos (2\pi t / T))$ and $\Delta = 0$.

5. Systematic errors

In this section, we shall only consider systematic errors, i.e. $\lambda = 0$. It suffices to work with pure states, instead of density matrices, satisfying the Schrödinger equation

\[
i \hbar \frac{d}{dt} |\psi(t)\rangle = (H_0(t) + \beta H_1)|\psi(t)\rangle.
\]

We define the systematic error sensitivity as

\[
q_s := -\frac{1}{2} \frac{\partial^2 P_2}{\partial \beta^2} \bigg|_{\beta = 0} = -\frac{\partial P_2}{\partial (\beta^2)} \bigg|_{\beta = 0},
\]

where $P_2$ is the probability to be in the excited state at the final time $T$.

Using perturbation theory up to $O(\beta^2)$, we obtain

\[
|\psi(T)\rangle = |\psi_0(T)\rangle - \frac{i}{\hbar} \beta \int_0^T dt \hat{U}_0(T, t) H_1(t)|\psi_0(t)\rangle - \frac{1}{\hbar^2} \beta^2 \int_0^T dt \int_0^t dt' \hat{U}_0(T, t) H_1(t) \hat{U}_0(t, t') H_1(t')|\psi_0(t')\rangle + \cdots,
\]

where $|\psi_0(t)\rangle$ is the unperturbed solution and $\hat{U}_0$ the unperturbed time evolution operator. We assume that the error-free ($\beta = 0$) scheme works perfectly, i.e. $|\psi_0(T)\rangle = e^{i\nu}|2\rangle$ with some real $\nu$. Then

\[
P_2 = |\langle 2 |\psi(T)\rangle|^2 = \langle \psi(T)|\psi_0(T)\rangle \langle \psi_0(t)|\psi_0(t)\rangle \approx 1 - \beta^2 \left| \int_0^T dt \langle \psi_\perp(t)| H_1(t)|\psi_0(t)\rangle \right|^2,
\]

because $\hat{U}_0(s, t) = |\psi_0(s)\rangle\langle \psi_0(t)| + |\psi_\perp(s)\rangle\langle \psi_\perp(t)|$, where $\langle \psi_\perp(t)|\psi_0(t)\rangle = 0$ for all times and $|\psi_\perp(t)\rangle$ is also a solution of the Schrödinger equation, see (9). From this we obtain the systematic-error sensitivity value

\[
q_s = \frac{1}{\hbar^2} \left| \int_0^T dt \langle \psi_\perp(t)| H_1(t)|\psi_0(t)\rangle \right|^2.
\]

5.1. Example: $\pi$ pulse

Let $\Delta = 0$, $\Omega(t) = |\Omega(t)| e^{i\omega}$ and $\int_0^T dt |\Omega(t)| = \pi$, which correspond to a $\pi$ pulse. Then we obtain that $H_0 = H_1$ and an analytical solution exists,

\[
P_2 = \frac{1}{2} - \frac{1}{2} \cos \left( (1 + \beta) \int_0^T dt |\Omega(t)| \right) = \frac{1}{2} - \frac{1}{2} \cos \left( (1 + \beta)\pi \right).
\]

It follows that $q_s = \pi^2 / 4$ independently of the time duration $T$.

The excitation probability versus systematic noise $\beta$ is shown in figure 4. As an example we are looking at the MNS-optimal protocol of the previous section (green, dashed line). It has the systematic-error sensitivity $q_s = \frac{\pi^2}{4} \approx 2.47$, which is equal for all $\pi$ pulses. Even if the protocol is maximally robust concerning amplitude noise, it is very sensitive to systematic errors.
Figure 4. Excitation probability $P_2$ versus systematic-error parameter $\beta$: zero systematic-error sensitivity (ZSS)-optimal protocol (blue, dashed-dotted line), transitionless protocol (red, solid line) and MNS-optimal protocol (green, dashed line). Additional parameters for the transitionless protocol are provided in figure 1.

5.2. Example of a transitionless shortcut

We again look at the example of a transitionless shortcut based on the sinusoidal model which was examined in subsection 4.2. An example of the excitation probability versus systematic noise $\beta$ is shown in figure 4 (red solid line). The transitionless shortcut based on the sinusoidal model is more stable concerning systematic errors than any $\pi$ pulse.

Figure 5 shows the systematic-error sensitivity for the transitionless-based protocol for different values of $\delta_0$ and $\Omega_0$. Again, the protocol takes as a reference the sinusoidal model (22). Note that the systematic-error sensitivity $q_S$ for any $\pi$ pulse corresponds to the upper $x-y$ plane in this figure. This means that for all the parameters shown, the transitionless shortcut is less sensitive (i.e. more stable) concerning systematic errors than any $\pi$ pulse.

5.3. Optimal scheme

To find an optimal scheme we shall use the invariant-based technique. The pure state $|\psi(t)\rangle$ can be parameterized as in (8). Let $\Theta(t)$, $\alpha(t)$ and $\gamma(t)$ be given. The boundary values should be $\Theta(0) = 0$ and $\Theta(T) = \pi$. We get the functions in the Hamiltonian leading to this solution from (11)–(13). Using (9) for the solution orthogonal to (8), i.e. $\langle \psi_\perp | \psi \rangle = 0$ for all times, the expression for the systematic error sensitivity is now

$$q_S = \frac{1}{4} \int_0^T dt \left[ e^{-i\gamma} \cos \Theta \sin \Theta + e^{-i\gamma} \Theta \right]^2$$

$$= \frac{1}{4} \int_0^T dt \left[ e^{-i\gamma} \frac{d}{dt} \left( \cos \Theta \sin \Theta + e^{-i\gamma} \Theta \right) \right]^2,$$

New Journal of Physics 14 (2012) 093040 (http://www.njp.org/)
where we have applied partial integration in the last step taking into account the boundary values \( \Theta(0) = 0 \) and \( \Theta(T) = \pi \). The expression can be further simplified and we obtain finally

\[
q_S = \left| \int_0^T dt \ e^{-i\gamma(t)\sin^2(\Theta)} \right|^2.
\]

In the special case when \( \gamma(t) \) is constant in time, we obtain \( q_S = \frac{\pi^2}{4} \) independently of \( \Theta(t) \). With the choice \( \alpha(t) \) constant we recover the \( \pi \) pulse.

The minimum of \( q_S \) is clearly achieved if \( q_S = 0 \). In the following we will show that there are protocols which fulfil this condition, i.e. protocols maximally stable with respect to systematic errors. We will give an example class which fulfils \( q_S = 0 \). Let

\[
\gamma(t) = n \ (2\Theta - \sin(2\Theta)).
\]

For this choice of \( \gamma \) we obtain

\[
q_S = \frac{\sin^2(n\pi)}{4n^2}.
\]

So, for \( n = 1, 2, 3, \ldots \), we obtain protocols fulfilling \( q_S = 0 \). Note that in the limit of \( n \to 0 \) (i.e. \( \gamma \to 0 \)), we obtain \( q_S \to \frac{\pi^2}{4} \), which is consistent with the previous paragraph. The functions in the Hamiltonian in this case are

\[
\Omega_\delta = (4n \cos \alpha \sin^3 \Theta - \sin \alpha) \ \dot{\Theta},
\]
\[
\Omega_1 = (4n \sin \alpha \sin^3 \Theta + \cos \alpha) \ \dot{\Theta},
\]
\[
\Delta = -4n \cos \Theta \sin^2 \Theta - \dot{\alpha}.
\]

Note that this class of protocols might not be the only ones fulfilling \( q_S = 0 \). There is still some freedom left. For example, one could in addition require that \( \Delta = 0 \) or \( \Omega_1 = 0 \). In the following we will look at the second condition, i.e. \( \Omega_1 = 0 \) for all \( t \). This leads to \( \alpha(t) = -\arccot(4n \sin^3 \Theta) \). In addition, there is the freedom to chose \( \Theta(t) \) with \( \Theta(0) = 0, \ \Theta(T) = \pi \).
Figure 6. ZSS-optimal protocol: Rabi frequency $\Omega_R$ (red, solid line) and detuning $\Delta$ (blue, dashed line).

We set $n = 1$ and $\Theta(t) = \pi t / T$; we call the resulting scheme the ‘zero systematic-error sensitivity’ (ZSS)-optimal protocol. Its Rabi frequency and its detuning are then

$$\Omega_R = \frac{\pi}{T} \sqrt{1 + 16 \sin \left( \frac{\pi t}{T} \right)^6},$$

$$\Delta = -8 \frac{\pi}{T} \sin \left( \frac{\pi t}{T} \right) \sin \left( \frac{2\pi t}{T} \right) \frac{1 + 4 \sin \left( \frac{\pi t}{T} \right)^6}{1 + 16 \sin \left( \frac{\pi t}{T} \right)^6},$$

and are shown in figure 6.

6. Systematic and amplitude-noise errors

Finally, we will consider both types of errors together. Optimal schemes in this case would depend on the ratio between amplitude-noise error and systematic error in the experiment. We will just examine numerically the behavior of some protocols with respect to amplitude noise and systematic error. Specifically, we compare the MNS-optimal protocol, the ZSS-optimal protocol and the example of a transitionless shortcut studied before, see figure 7. The figure shows that the different optimal schemes perform better than the other one depending on the dominance of one or the other type of error.

There are other types of error, for example, quantum noise leading to dephasing. In that case, the Bloch equation would be

$$\frac{d}{dt} \vec{r} = (\hat{L}_0 - \kappa^2 \hat{L}_3) \vec{r},$$

where

$$\hat{L}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$
**Figure 7.** Probability $P_2$ versus noise error and systematic error parameter; (a) transitionless protocol (red), ZSS-optimal protocol (blue), MNS-optimal protocol (green); the same result as contour plots: (b) transitionless protocol, (c) ZSS-optimal protocol and (d) MNS-optimal protocol. Additional parameters for the transitionless protocol are provided in figure 1.

**Figure 8.** Probability $P_2$ versus dephasing strength $\kappa$: transitionless protocol (red, solid line), ZSS-optimal protocol (blue, dashed line) and MNS-optimal protocol (green, dotted line). The parameters for the transitionless protocol are given in figure 1.

This type of error will be studied in detail in a future publication. Nevertheless, as an outlook we show in figure 8 the excitation probability $P_2$ for the three schemes versus different values of the dephasing strength $\kappa$. All three schemes are very stable concerning dephasing error.
To summarize, in this paper we have examined the stability of different fast protocols for exciting a two-level system with respect to amplitude-noise error and systematic errors. First we looked at the noise error alone and introduced a noise sensitivity. We showed that a special type of $\pi$ pulse is the optimal protocol with MNS. Then we looked at the systematic error alone and introduced a systematic error sensitivity. We showed that there are protocols for which this sensitivity is exactly zero. Finally, we looked at the general case with noise and systematic errors together.

Future work will involve extending the present results to different types of noise and perturbations. The existence of a set of optimal solutions for systematic errors also opens the way to further optimization with respect to other variables of physical interest.

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Appendix. Derivation of the master equation for amplitude-noise error

The evolution of the quantum state with amplitude noise can only be described by a master equation \[ \frac{\hbar}{i} \\frac{d}{dt} \psi(t) = \left( H_{01} + \lambda H_2 \frac{dW_t}{d\xi(t)} \right) \psi(t), \] where $dr$ is the infinitesimal time step and $dW_t$ is the corresponding noise increment in the Ito sense. The properties of such noise are: $\langle dW_t \rangle = 0$, $\langle dW_t^2 \rangle = dt$. If we expand in Taylor series (A.1) and keep terms up to first order in $dt$ and $dW$ (using the Ito calculus rules), we arrive at the following stochastic Schrödinger equation (SSE):

\[ |d\psi| = -\frac{i}{\hbar} H_{01} dt |\psi| - \frac{\lambda^2}{2\hbar^2} H_2^2 dt |\psi| - \frac{i\lambda}{\hbar} H_2 dW_t |\psi|. \] (A.2)

The master equation derived from this SSE is then (14).

An equivalent approach in the Stratonovich sense is to start from

\[ i \hbar \frac{d}{dt} \psi(t) = \left( H_{01} + \lambda H_2 \frac{dW_t}{d\xi(t)} \right) \psi(t), \] where $\xi(t)$ is heuristically the time derivative of the Brownian motion $W_t$. We have $\langle \xi(t) \rangle = 0$ and $\langle \xi(t) \xi(t') \rangle = \delta(t - t')$ because the noise should have zero mean and the noise at different times should be uncorrelated. If we average over different realizations and define $\rho(t) = \langle \rho_\xi \rangle$, then $\rho(t)$ is fulfilling (14). To show this, we define $\rho_\xi(t) = |\psi_\xi(t)\rangle \langle \psi_\xi(t)|$. We start from the dynamical equation for $\rho_\xi$, namely

\[ \frac{d}{dt} \rho_\xi = -\frac{i}{\hbar} [H_{01}, \rho_\xi] - \frac{i\lambda}{\hbar} [H_2, \xi \rho_\xi], \] (A.3)
which after averaging over the noise becomes
\[
\frac{d}{dt} \rho = -\frac{i}{\hbar} [H_{01}, \rho] - \frac{i\lambda}{\hbar} [H_2, \langle \xi \rho \xi \rangle]. \tag{A.4}
\]

Novikov’s theorem applied to white noise takes the form
\[
\langle \xi(t) F[\xi] \rangle = \left. \frac{1}{2} \delta F(s) \right|_{\delta \xi(s) = 0}. \tag{A.5}
\]

Using it, we obtain
\[
\langle \xi \rho \xi \rangle = -\frac{i\lambda}{2\hbar} [H_2, \rho],
\]
which leads to (14).

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