Robustness and Errors in Quantum Optimal Control

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We introduce a new approach to quantify the robustness of optimal control of closed quantum systems. Our theory allows to assess the degree of distortion that can be applied to a set of known optimal control parameters, which are solutions of an optimal control problem. The formalism is applied to an exactly solvable model and to the Landau-Zener model, whose optimal control problem is solvable only numerically. The presented method is of importance for any application where a high degree of controllability of the quantum system dynamics is required.

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The theory of optimal control (OC) that has been mathematically formulated in the last century by the seminal works of Pontryagin, Bellman, Kalman, Stratonovich 1,2 has been instrumental for the achievement of highly reliable electronic devices used to control, for instance, mechanical systems such as airplanes, cars, etc., but also to control chemical reactions or to design ultra-fast laser pulses for manipulating molecules (e.g., to break a certain bond while leaving other bonds intact 3), and today even to optimize (stochastic) financial analyses.

The topic has recently attracted the attention of physicists working in quantum information and computation science, because of the need to engineer tailored quantum information processing and matter. To this aim different numerical techniques have been devised in order to minimize (or maximize) some performance criterion or, alternatively called, objective functional. We mention the most used ones in open-loop quantum control: the Krotov iterative method 4, 5 and the gradient ascent pulse engineering algorithm 6. Although these are powerful tools, once the optimal solution of a particular control problem is found, there is no systematic way, to our knowledge, to give an assessment of the robustness of the obtained OC signal. A possible (empirical) approach relies on applying an arbitrary distortion to the OC solution and then looking at the error that it produces on the objective functional, or by selecting a region in the Hilbert space that is robust against noise (decoherence free-subspace) 7, whose existence follows from the symmetry properties of the noise.

The aim of this Letter is to provide a general method to quantify how robust a given OC scheme is and to which extent it can tolerate errors. Even though usually it is not possible to know analytically the OC pulse, we underscore that our philosophy is that the parameter obtained with some numerical algorithm is very close to the global optimum. More precisely, the error on the cost functional obtained with the numerically found OC pulse has to be much smaller than the error allowed by the process we are interested to optimize. Besides the interest on its own, we believe that our approach is of importance for experiments, where, typically, optimal pulses are extremely difficult to achieve. Indeed, our method can help to find a control signal that is experimentally more robust than the ideal OC pulse, while still able to satisfactorily fulfill the performance criterion we are interested in.

Let us briefly review what is the purpose and what are the methodologies adopted commonly in the quantum control research area concerning closed quantum systems and the link between OC theory and analytical mechanics. The usual problem is the engineering of a control Hamiltonian $\hat{H}(u_t)$, with $u_t \equiv u(t)$ being the control pulse, such that the initial state $|\psi_{in}\rangle$ at time $t = t_0$ of the quantum system under consideration is brought at time $t = T$ to some desired goal state $|\psi_{g}\rangle$ (see also Fig. 1). To this aim there are two techniques for searching optimal pulses at our disposal: the variational method and dynamical programming. In both cases the goal is the minimization of the cost functional

$$J[t_0, u_t, \psi_t] = G(\psi_T) + \int_{t_0}^{T} dt C(t, u_t, \psi_t) \quad (1)$$

Figure 1. (Color online) Pictorial representation of the optimal trajectory $|\psi_{f}\rangle$ (red-thick line) obtained with the OC pulse $u_{t}$ and trajectories (thin lines) for non-optimized control pulses. The shaded (green) area represents the portion of Hilbert space within which the cost functional $J \leq J'$ (see also text), that is, the subset of state vectors close to the goal state $|\psi_{g}\rangle$. 

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over all admissible control pulses $u_t$ and state trajectories $|\psi_1\rangle \equiv |\psi(t)\rangle$ given a certain initial state $|\psi_{in}\rangle$. Here by admissible we mean any $u_t$ for which the Schrödinger equation is well-defined and has a unique solution $|\psi_t\rangle$ given the initial condition $|\psi_{in}\rangle$. The first term on the r.h.s. of Eq. (4) is the terminal functional, e.g., the overlap infidelity $1 - |\langle \psi_f | \psi_T \rangle|^2$. The second term provides additional constraints on the control pulse $u_t$. In the variational method the additional constraint $\text{Re}\{\int_0^T dt [i\chi_t |\psi_t\rangle + i\chi_t \hat{H}(u_t)|\psi_t]\}$ is introduced, where we set $\hbar = 1$ and $|\chi_t\rangle$ is a Lagrange multiplier often referred to as costate, which ensures that the state $|\psi_t\rangle$ satisfies the Schrödinger equation. The search of an extremum of the cost functional produces a set of equations for the state, costate and the control pulse.

On the other hand, dynamical programming, based on the Bellman’s optimality principle [11], produces an equation, the so called Hamilton-Jacobi-Bellman equation, for the optimal cost $S(t, \psi_t) := \inf_{u_t} J(t, u_t, \psi_t)$. This equation is expressed in formally the same way as the Hamilton-Jacobi equation of classical mechanics, but with the difference that it is propagated backwards in time. The role of the Hamilton function in classical mechanics is played in control theory by the (quantum) Pontryagin Hamiltonian $H(\chi, \psi) := \sup_{u_t} \{\text{Re}[i\chi_t \hat{H}(u_t)|\psi_t]\} - C(t, u_t, \psi_t)$ [11]. From the Hamilton-Jacobi-Bellman equation it is possible to retrieve the equations of motion for the state and the costate, the same as in the variational approach, which look, given the aforementioned Pontryagin Hamiltonian, formally as the Hamilton equations for the phase space variables $(q, p)$ in analytical mechanics.

Motivated by this analogy between OC theory and analytical mechanics we can view the cost functional as an “action functional”. Indeed, in analogy to the Hamilton’s principle where the actual evolution of a classical system is an extremum of the action functional, which produces the well-known Euler-Lagrange equations of motion, an extremum of $J$ produces the OC equations for the state and the costate.

Now, our goal is to provide a program that enables us to quantify the robustness of an OC pulse $u^o_t$. The first step is to fix the desired cost, $J$, that the system (at least) has to attain. Since the advantage of optimizing quantum dynamics is connected with the possibility of reaching $|\psi_k\rangle$ by exploiting the interference of several paths in the space of control parameters $U$, our next step is to define a path integral in such a space. To this aim, we introduce the weight $K = \sum_{u_t} e^{\frac{1}{\alpha_t} J(u_t, \psi_t)}$ on the space $U$. The form of this weight resembles the Feynman propagator, which is motivated by the previous discussed analogy between analytical mechanics and OC theory. The numerical factor $\alpha_t$, which we shall refer to “infidelity tolerance”, has the following property: when $J$ approaches the minimum of $J$, then $\alpha_t \to 0$. Hence, $\alpha_t$ is the analogous of $\hbar$ in Feynman path integral. Indeed, when $\alpha_t \to 0$ we retrieve the OC equations for the state and the costate we mentioned before. Besides this, $\alpha_t$ must be unique for a given OC problem, regardless of the form of the distortion $\delta u_t = u_t - u^o_t$, or else our method would be ineffective. Finally, the last step of our procedure is to define a suitable norm in $U$ for $\delta u_t$, by means of $K$, in order to afford a quantitative appraisal of the robustness of an OC pulse.

To be specific let us set, for the sake of simplicity, $t_0 = 0$ and consider only one control pulse $u_t$. We also assume that the state $|\psi_t\rangle$ obeys the Schrödinger equation with the time-dependent Hamiltonian operator $\hat{H}(u_t)$ and initial condition $|\psi_0\rangle \equiv |\psi(0)\rangle$. Contrarily to [11], where the state $\psi$ is an independent variable, hereafter we render explicit the dependence of $\psi$ on the control parameter $u_t$. Thus, we introduce the reduced cost functional $J'[u] := J[u, \psi(u)]$. Then by performing the Taylor expansion of $J'[u]$ around $u^o_t$ to second order in $\delta u_t$ we obtain

$$J'[u_t] \simeq J'[u^o_t] + \frac{1}{2} \Delta^2 J'[u^o_t, \delta u_t, \delta u_t] + O(\| \delta u_t \|^3).$$

Here $\| \cdot \|$ is some norm in $U$, whereas $J'[u^o_t]$ is the minimum, which, without loss of generality, we will set to zero. In Eq. (2) $\Delta J'[u^o_t, \delta u_t, \delta u_t]$, $\delta u^T = [\delta u_2, \delta u_N]$, where $\delta u^T$ is the transpose of the vector $\delta u = (\delta u_2, \ldots, \delta u_N)$ and the time interval $[0, T]$ is divided in $N - 1$ equal parts $\Delta t = T/(N - 1)$. The Hessian $H$ is a real, symmetric, and positive defined matrix, and therefore it can be diagonalized. Additionally, we assume the boundary conditions $\delta u_0 = \delta u_T = 0$, that is, the values $u_0$ and $u_T$ are fixed.

Obviously, the norm in $U$ has to be a monotonic function of $J'$. A suitable choice for such a norm is given by: $\| J'[u] \| = \int [D|u|] J'[u_t] \exp(\frac{1}{\alpha_t} J(u_t))]$ with $\int [D|u|] = \lim_{N \to \infty} \int [D|u|] = N \to \infty \int [D|u|] = \int [D|u|]$. This norm is indeed an “average” in $U$ of the reduced cost functional itself with the exponential function being a “probability distribution”. Close to the optimal solution we can approximate $J'$ with its second order expansion, and therefore we can write

$$J' \simeq \int [D|u|] \Delta^2 J'[u^o_t, \delta u_t, \delta u_t] e^{\frac{1}{\alpha_t} \Delta^2 J[u^o_t, \delta u_t, \delta u_t]}.$$  

Hence the discretized version of the norm becomes

$$\int [D|u|] \simeq \int \frac{\sqrt{\pi}}{2} \int \frac{\sqrt{2}}{\lambda_k} \sum_{\lambda_k}^{N - 2} \sqrt{N_k} e^{\frac{1}{\alpha_t} \Delta^2 J'[u^o_t, \delta u_t, \delta u_t]} \int [D|u|]$$

where $N_k^{-1} = \int [e^{i\lambda_k \Delta t} / (2\alpha)]$ are normalization factors, and $\lambda_k$ for $k = 1, \ldots, N - 2$ are the eigenvalues of $H$. The above formula makes good sense, because when $\alpha_t \to 0$ also $\int [D|u|] \to 0$. 
In order to apply the above outlined formalism to some concrete example we shall consider hereafter \( J'[u_t] = 1 - F(\psi_T) \), with \( F(\psi_T) = |\langle \psi_T | \psi_T \rangle|^2 \). We note that the state \( |\psi_T \rangle \) is implicitly depending on the whole history of \( u_t \forall t \in [0, T) \). Assuming that \( F(u_t, \psi(t)) \) is a differentiable functional of its arguments we have

\[
J'[u_t] = 1 - F(\psi_0) + 2 \int_0^T dt \Im[\langle \psi \delta \psi_t | H(u_t) | \psi_0 \rangle], \tag{5}
\]

The most difficult part of the outlined program is the computation of the functional derivative of the integrand in Eq. (5), namely \( \Delta^2 J' \) in (2), that is, the Hessian matrix \( \mathbf{H} \). To this aim we have two possibilities at our disposal: either we estimate \( \mathbf{H} \) by means of the Broyden-Fletcher-Goldfarb-Shanno formula [11] or we compute the first and second derivatives of the state \( |\psi \rangle \) with respect to the control \( u_t \). We choose the latter approach, where we have to solve the following equations

\[
\begin{align*}
\partial_t |\psi^2 \rangle & + i \hat{H}(u_t^2)|\psi^2 \rangle = -2i\delta \hat{H}(u_t^2)|\psi \rangle - i(\delta^2 \hat{H}(u_t^2))|\psi_2 \rangle, \\
\partial_t |\psi \rangle & + i \hat{H}(u_t^2)|\psi \rangle = -i(\delta \hat{H}(u_t^2))|\psi_2 \rangle,
\end{align*}
\]

which apply to any quantum closed system. Here \( |\psi_2 \rangle \) is the solution of the Schrödinger equation for \( \hat{H}(u_t^2) \), and \( \delta \hat{H}(u_t^2), \delta^2 \hat{H}(u_t^2) \) are the Gateaux derivatives of the control Hamiltonian (defined as: \( \delta \hat{H} \equiv \frac{d\hat{H}[u_t+\alpha \delta u_t]}{d\alpha} |_{\alpha=0} \)), which are analytically computable. By solving these equations we are able to determine the matrix \( \mathbf{H} \).

Let us first apply our method to a simple exactly solvable model. We consider the transport of a particle in a movable one-dimensional harmonic trap potential, for which the OC pulse and the functional dependence of the state on the controller are analytically known [12]. The control Hamiltonian is given by \( \hat{H}(u_t) = \frac{1}{2}(\hat{p}^2 + x^2 - U_0)^2 \) with \( [\hat{x}, \hat{p}] = i \) (we use harmonic oscillator units). We focus our attention on the ground state, that is, when we consider a particle over the distance \( \Delta x \) in a time \( T \) such that \( \psi_T(x) = e^{i\varphi} \phi_0(x - \Delta x) \equiv \phi_0(x) \), where \( \varphi \) is an unimportant phase factor and \( \phi_0(x) \) is the Gaussian harmonic oscillator ground state wavefunction. Thus, our goal is to find a prescription such that when the OC pulse is perturbed the system has to reach at least the a priori fixed value of fidelity \( F \in [0, 1] \).

In Ref. [12] the analytic solution for the time evolved state is provided. This enables us to compute analytically the Gateaux derivatives of the state of the system without the need of solving (4). In Fig. 2(a) we show results for a distortion given by \( \delta u_t = a \sin(\kappa 2\pi t/T) u_0^2 \), with \( u_0^2 \) being the OC pulse of Ref. [12] [see Eq. (5) therein]. Such simple distortion modulates the OC pulse at the rate \( \kappa \) and gives a direct quantitative measure of the distortion degree applied to \( u_0^2 \): the larger \( a \) is, the larger the infidelity. Thus, Fig. 2(a) shows which is the largest admissible value of \( a \) for a fixed value of the (reduced) cost functional, whereas in the inset we show the deviation from the linear behaviour of \( \Delta^2 J'/2 \) for \( \kappa = 1 \).

Now we write the cost functional as \( 2J'[u_t] \approx \delta u_0 \mathbf{H} \delta u_0^T \). In this specific example it turns out, numerically, that the matrix elements of \( \mathbf{H} \) are of the form \( H_{nk} = h + \delta H_{nk} \) with \( h, \delta H_{nk} \in \mathbb{R} \) such that \( \delta H_{nk}/h \ll 1 \). This means that the matrix elements are almost equal to each other. The eigenvalue problem for such a matrix can be well approximated by \( \lambda = -\tilde{\lambda} \delta^2 \hat{H} \equiv \langle \Delta^2 \hat{H} | u_0^2, \delta u_t, \delta u_t^2 \rangle / \pi^2 \), with \( \tilde{\lambda} = (N - 2)\delta x^2 \). Thus, by defining \( \tilde{\lambda} \equiv \sum_{nk} H_{nk} (N - 2)^2 \), we get for the non-vanishing eigenvalue the simple expression \( \lambda_0 = (N - 2)\delta x^2 \). Given these remarks, the norm (4) reduces to \( \langle J' \rangle \approx \sqrt{\pi a^2 (\lambda^2)} \).

Finally, in order to determine \( \alpha_t \) we proceed in the following way: since the norm is the “average cost functional” and \( \alpha_t \) has to be unique, we simply use the inverted formula \( \alpha_t = [2\lambda_0 (\Delta^2 J'[u_0^2, \delta u_t, \delta u_t^2] / \pi]^{1/2} \) for a given choice of \( \delta u_t \). We tested, however, that different kinds of distortions produce (practically) the same curve as the one shown in Fig. 2(b). This is easily understood, since what is relevant for the overlap infidelity terminal functional is the final state \( |\psi_T \rangle \). Secondly, we perform a fit of the obtained curve for \( \alpha_t \) as a function of the overlap infidelity. For the present example, showed in
state. For such a control problem both the iterative method \[1, 13\]. We then proceed on, as in the former example, by determining the infidelity tolerance \(\ell\). Analogously to the former example, only the realizations of \(\delta u_0\) that fulfill \(\delta u_0^2 \leq \ell(0.99)\) have an infidelity below 1%.

In conclusion we have presented a method to assess the robustness of solutions to OC problems. The method will be a powerful tool for experimentalists in order to evaluate errors, and therefore to design experiments robust against source of noise. For instance, to estimate how much the schemes for realizing quantum gates are robust against imperfections of the optimal pulse shape. Our method can be applied to both known error models and to evaluate unknown errors such as random telegraphic noise. Besides this, we plan to extend our formalism to dissipative quantum systems (e.g., systems governed by the Born-Markov master equation).

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**References**


[7] For instance, the “laser electric field fluence” with \(C(u_t) = u_t^2\), where \(u_t\) is an electric field amplitude.


