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Abstract

We present a new formulation of monotonically convergent algorithms which allows to optimize both the control duration and the laser fluence. A standard algorithm designs a control field of fixed duration which both brings the system close to the target state and minimizes the laser fluence, whereas here we include in addition the optimization of the duration in the cost functional. We apply this new algorithm to the control of spin systems in Nuclear Magnetic Resonance. We show how to implement CNOT gates in systems of two and four coupled spins.

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I. INTRODUCTION

The optimal control of quantum systems is a long-standing goal [1–3] which remains very attractive both from a practical and a fundamental point of views [4, 7, 8]. By finding the optimal balance between the minimization of the distance to the target state and the minimization of the energy of the laser, the optimal solution allows to bring the system close to the target state while avoiding parasitic phenomena due to a too large laser fluence. In this context, the control duration is also a crucial parameter which has to be taken into account in the optimization process. For instance, a too long duration could be problematic if other concurrent physical or chemical processes with the same time scale occur during the control. This question is particularly interesting in quantum computing where coherence has to be preserved [9]. Since a control field cannot generally fully compensate the dissipation effects [35], a too long interaction of the system with the environment can destroy its coherence and the quantum superposition or the entanglement produced by the control.

Solving time-optimal control problems remains however a challenging task. One way is to use the Pontryagin maximum principle and geometric optimal control theory [10, 11]. However, such techniques can only be applied for the moment to small dimensional quantum problems with very few energy levels [12, 14–17]. On the other hand, monotonically convergent algorithms are an efficient way to solve optimal control problems and have been widely used in the control of chemical and physical processes since the pioneering papers by Tannor et al. [18] and Rabitz et al. [19] which were based on the work of Krotov [36]. This approach can be applied to very different and large quantum systems (See e.g. [20–24]) and to a variety of non-standard situations such as the nonlinear interaction between the system and the control field [25, 26] or to take into account spectral constraints on the optimal solution [27, 28]. Up to now, however, these algorithms have generally be used with a cost penalizing the laser fluence and a fixed control duration. By construction of these algorithms, a formulation in terms of a time-optimal control, i.e. with a duration which is not fixed, is a very difficult question since these methods imply the backward propagation of the adjoint state from the final time of the control. Other time-optimal control algorithms have already been proposed in [31, 32], but these propositions differ from our approach in the sense that a second Lagrange multiplier on the control duration (in addition of the adjoint state) is added. This leads to a more complicated algorithm than the one proposed below.

We present in this paper a new formulation of monotonically convergent algorithms with a cost penalizing both the laser fluence and the control duration, which allows us to find the best compromise between these two parameters. Using a rescaling of time, we first rewrite the optimal equations on a fixed time interval independent on the control duration T, which appears as a new parameter in the time-dependent Schrödinger equation. We then consider a monotonic iterative algorithm whose each step is decomposed into two substeps consisting in an optimization of the energy of the field with T fixed and an optimization of the time T with a fixed control field. The first substep is realized through a standard monotonically convergent algorithm, while a gradient or another discrete optimization procedure is used for the second substep. We impose that each substep increases the cost functional leading thus to a monotonic algorithm.

To test the efficiency of this approach, we consider the control of spin systems [5], and in particular the implementation of quantum gates in such systems. Different technologies have been developed so far to exploit the powerful of quantum computing. One of the most promising solution is Nuclear Magnetic Resonance (NMR) [30]. The control technology developed over the past fifty years allows the use of sophisticated control fields and permits the implementation of complex quantum algorithms such as the Deutsch-Jozsa and the Grover ones [6]. NMR is therefore an ideal testbed to experiment new ideas in quantum control. In this paper, we show how to implement two and four qubits CNOT gates. These different numerical computations allow to extract the main properties of our algorithm and to highlight the differences with respect to a standard approach.

The paper is organized as follows. In Sec. II, we describe the new monotonically algorithm for pure state quantum systems. The proof of its monotonic character is established. Section III is devoted to the application of this approach in a two and four spin systems in order to implement CNOT gates. We conclude in Sec. IV.

II. TIME-OPTIMAL CONTROL ALGORITHMS

We present in this section the algorithm in a general setting for pure quantum states. The formalism can be straightforwardly extended to mixed-state quantum systems [21] or to the control of evolution operators [29]. It is this latter generalization that will be used in Sec. III for the implementation of quantum gates. We consider the maximization of the projection

onto a target state, but the algorithm could be equivalently defined for maximizing the expectation value of a given observable.

A. Methodology

Let $|\phi_0\rangle$ and $|\phi_f\rangle$ be the initial and target states of the dynamics. We consider the time-optimal control problem of maximization of the cost functional $J_T(E_T)$ over the control duration T and the control field E_T. Note that the subscript T is added in this paper to any quantity depending upon this time. The functional J_T is defined by

$$J_T(E_T) = 2\Re[\langle\psi_T(T)|\psi_f\rangle] - \alpha \int_0^T E_T^2(t)dt \tag{1}$$

where α is a positive parameter which weights the relative importance of the energy of the control field with respect to the projection onto the target state. $\Re[\cdot]$ is the real part of a complex number. The state $|\psi_T(t)\rangle$ of the system satisfies the time-dependent Schrödinger equation which is written in units such that $\hbar = 1$:

$$i\frac{\partial}{\partial t}|\psi_T(t)\rangle = (H_0 - \mu E_T(t))|\psi_T(t)\rangle \tag{2}$$

with as initial condition $|\psi_T(0)\rangle = |\phi_0\rangle$. The Hamiltonian H_0 is the field-free Hamiltonian and the operator μ describes the interaction between the system and the control field, which is assumed to be linear.

The first step of the approach is to define a fixed time interval, for instance $[0, 1]$. We consider for that purpose the time rescaling $s = t/T$. Introducing $|\psi(s)\rangle = |\psi_T(s \cdot T)\rangle$ and $E(s) = E_T(s \cdot T)$, we obtain from Eq. (2) that

$$i\frac{\partial}{\partial s}|\psi(s)\rangle = T(H_0 - \mu E(s))|\psi(s)\rangle \tag{3}$$

with the initial condition $|\psi(0)\rangle = |\phi_0\rangle$. The cost functional is also changed by the time rescaling and becomes

$$J(E) = 2\Re[\langle\psi(1)|\psi_f\rangle] - \alpha T \int_0^1 E^2(s)ds. \tag{4}$$

The new optimal control problem consists now in maximizing the cost functional J with respect to the control field E and the time T which plays here the role of a parameter. The control duration is fixed to 1.

B. Monotonically algorithm

The algorithm is decomposed into two substeps. We alternatively optimize the functional J with respect to the control field E by a standard monotonic algorithm and with respect to the duration T by a discrete procedure such as a gradient method. We prove that the cost increases at each step of the algorithm.

a. Optimization of the control field. We introduce the triplets $(|\psi(t)\rangle, E(t), T)$ and $(|\tilde{\psi}(t)\rangle, \tilde{E}(t), T)$ corresponding to the initial and final states of this substep of the algorithm. The variation of the cost is given by:

$$\begin{aligned}\Delta J &= J(\tilde{E}) - J(E) \\ &= 2\Re[\langle\tilde{\psi}(1) - \psi(1)|\psi_f\rangle] - \alpha T \int_0^1 (\tilde{E}^2(s) - E^2(s) ds.\end{aligned}$$

We introduce the adjoint state $|\chi(t)\rangle$ which satisfies

$$i\frac{\partial}{\partial s}|\chi(s)\rangle = T(H_0 - \mu E(s))|\chi(s)\rangle \tag{5}$$

with the final condition $|\chi(1)\rangle = |\phi_f\rangle$. We then have

$$\Re[\langle\tilde{\psi}(1) - \psi(1)|\phi_f\rangle] = \Re[\langle\tilde{\psi}(1) - \psi(1)|\chi(1)\rangle] \tag{6}$$

which can be transformed into

$$\Re[\langle\tilde{\psi}(1) - \psi(1)|\phi_f\rangle] = \Re\big[\int_0^1 ds[\langle\frac{\partial}{\partial s}\chi|\tilde{\psi} - \psi\rangle + \langle\chi|\frac{\partial}{\partial s}(\tilde{\psi} - \psi)\rangle]\big]. \tag{7}$$

Using Eqs. (3) and (5), one deduces that

$$\Re[\langle\tilde{\psi}(1) - \psi(1)|\phi_f\rangle] = 2T\Im[\int_0^1 ds\langle\chi|\mu(\tilde{E} - E)|\tilde{\psi}\rangle]. \tag{8}$$

One finally arrives to

$$\Delta J = \alpha T \int_0^1 ds(E - \tilde{E})(E + \tilde{E} + \frac{2}{\alpha}\Im[\langle\chi|\mu|\tilde{\psi}\rangle]). \tag{9}$$

Knowing $E(s)$, the choice $\tilde{E} = -\Im[\langle\chi|\mu|\tilde{\psi}\rangle]/\alpha$ ensures that $\Delta J \geq 0$ for this substep. This part of the algorithm can be summarized as follows. Starting from the quadruplet $(|\psi(s)\rangle, |\chi(s)\rangle, E(s), T)$, we construct the quadruplet of the next sub-iteration by propagating backward the adjoint state $|\tilde{\chi}(s)\rangle$ from $|\phi_f\rangle$ with the field $E(s)$. We then propagate forward the state $|\tilde{\psi}(s)\rangle$ from $|\phi_0\rangle$ with the field $\tilde{E}(s)$ which is computed at the same time by the relation $\tilde{E}(s) = -\Im[\langle\tilde{\chi}(s)|\mu|\tilde{\psi}(s)\rangle]/\alpha$.

b. Optimization of the control duration. At this stage of the algorithm, we consider the triplets $(|\psi(s)\rangle, E(s), T)$ and $(|\tilde{\psi}(s)\rangle, E(s), \tilde{T})$. We recall that the state $|\tilde{\psi}(s)\rangle$ satisfies

$$i\frac{\partial}{\partial s}|\tilde{\psi}(s)\rangle = \tilde{T}(H_0 - \mu E(s))|\tilde{\psi}(s)\rangle. \tag{10}$$

We compute the variation of the cost functional ΔJ which is equal to:

$$\Delta J = 2\Re[\langle\tilde{\psi}(1) - \psi(1)|\psi_f\rangle] - \alpha(\tilde{T} - T)\int_0^1 E^2(s)ds. \tag{11}$$

Introducing the adjoint state $|\chi(s)\rangle$ whose dynamics is governed by Eq. (5), one obtains after similar computations as for the previous case that

$$\Delta J = \alpha(T - \tilde{T})\int_0^1 dsE(s)(\frac{2}{\alpha}\Im[\langle\chi|\mu|\tilde{\psi}\rangle] + E(s)). \tag{12}$$

The parameter $\tilde{T}$ has to be chosen such that $\Delta J \geq 0$. A solution consists in using a gradient method by noting that

$$\nabla_T J = -\alpha\int_0^1 dsE(s)(\frac{2}{\alpha}\Im[\langle\chi|\mu|\psi\rangle] + E(s)). \tag{13}$$

We define the new time $\tilde{T}$ from the preceding one as:

$$\tilde{T} = T - r\nabla_T J(E(s), T), \tag{14}$$

where r is a real parameter. We choose numerically r small enough to ensure the monotonicity of the cost functional. The computation of the optimal value of r requires however several new propagations to determine the cost J since the evolution of $|\tilde{\psi}\rangle$ (needed to calculate $\langle\tilde{\psi}(1)|\psi_f\rangle$) depends on the value of $\tilde{T}$ (see Eq. (10)). Other methods ensuring the monotonic behavior of the cost can be used for this substep as the following procedure. In this approach, we define the new duration $\tilde{T}_k$ as a function of the old duration T_k as follows:

$$\tilde{T}_k = (1 + a)T_k$$

where a is a small positive or negative parameter. Practically, we can choose e.g. $a = \pm 10^{-3}$, but this value can also be adjusted through the computation. This leads to two new costs $\tilde{J}_k^+$ and $\tilde{J}_k^-$. The final time at step k is the time associated to the maximum value between $\tilde{J}_k^+$, $\tilde{J}_k$ and $\tilde{J}_k^-$. This method has the advantage over the gradient approach to limit at each step the number of propagations of Eq. (3) to 2. This point can be interesting when very heavy computations are considered. This systematic procedure has been used in the numerical examples of Sec. III. In particular cases, we have checked that the gradient and this systematic approach give equivalent results.

III. CONTROL OF SPINS SYSTEMS

A. Description of the model

The principles of control in NMR are detailed in different books and review articles. Here we only give a brief account needed to introduce the model used [5]. We consider the control of a system of coupled spins by different magnetic fields acting as local controls on each spin. This means that each field only controls one spin and does not interact with the others, i.e. the spins are assumed to be selectively addressable. This hypothesis has the advantage to render the system completely controllable. Similar models have been used in numerical studies analyzing the realization of quantum algorithms in NMR [33].

More precisely, we introduce a system of n coupled spins whose evolution is described by the following Hamiltonian:

$$H = H_0 + \sum_{j=1}^{n} (u_{jx} H_{jx} + u_{jy} H_{jy}),$$

the couplings being given by:

$$H_{jx} = \sigma_{jx},\ H_{jy} = \sigma_{jy}$$

where the operators (σ_{jx}, σ_{jy}) are Pauli matrices which only act on the jth- spin. We assume that the free evolution Hamiltonian H_0 is associated to the topology of a chain of coupled spins with only nearest-neighbor interactions. The corresponding Hamiltonian is given by:

$$H_0 = \sum_{j=1}^{n-1} \sigma_{jz} \otimes \sigma_{j+1;\ z},$$

where the approximation is valid in heteronuclear spin systems if the coupling between the spins is small with respect to the frequency shifts [5]. The coupling between the spins is taken to be uniform and equal to 1. The different equations being linear, other couplings could be considered from a standard rescaling of the time and of the amplitude of the control fields. Note that the algorithm could also be used with different couplings between the spins.

B. Optimal implementation of a CNOT gate

Our goal is to apply the time-optimal control algorithm to implement a $C^{n-1}NOT$ gate (Controlled-Not) in a system of n qubits with $n = 2$ or 4. A $C^{n-1}NOT$ gate is a gate in

which the target qubit flips if and only if the $(n-1)$ control qubits are equal to 1. For $n=2$, the $CNOT$ transformation is represented by the unitary operator U_{CNOT} which can be written as:

$$U_{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

The logical states involved in a $C^{n-1}NOT$ gate can be mapped onto the spin states in different ways. A straightforward and natural way used in this paper to map the logical states onto the spin states is to encode the first qubit in the first spin, the second qubit in the second spin, and so on if more than two spins are considered.

To implement quantum gates, we formulate the control problem in terms of evolution operators $U(t)$. This means that the objective of the control is to reach the target state U_{CNOT}, while optimizing the control duration and the energy of the fields. The time-optimal monotonically convergent algorithm for evolution operators can be sketched along the same way as for the wave function case of Sec. II. This algorithm can be obtained by substituting the wave function $|\psi_T(t)\rangle$ by $U_T(t)$, and the scalar product $\langle\psi(t)|\chi(t)\rangle$ by $\mathrm{Tr}[U\dagger V]$ where $V(t)$ is the adjoint propagator. The corresponding cost functional is given by:

$$J(E) = 2\Re\big[\mathrm{Tr}[U_{CNOT}U_T(T)]\big] - \alpha\int_0^T E_T^2(t)dt, \tag{15}$$

the evolution operator $U_T(t)$ satisfying the Schrödinger equation

$$i\frac{\partial U_T(t)}{\partial t} = (H_0 - \mu E_T(t))U_T(t). \tag{16}$$

Note that, in the example considered, 2^n fields are simultaneously optimized. The efficiency of the process is measured by the projection $P = \frac{1}{2^n}\Re\big[\mathrm{Tr}[U_{CNOT}U_T(T)]\big]$.

From a numerical point of view, two different parameters, α_0 and $E_0(t)$, have to be adjusted when using this algorithm. These parameters do not play the same role since α is a parameter characteristic of the algorithm, while $E_0(t)$ is the initial field used to initiate the optimization process. More precisely, we assume that the parameter α depends on time and can be written as $\alpha(t) = \alpha_0 \sin^2(\pi t/T)$ where α_0 is a constant. This switching function is introduced to provide a smooth on and off switch of the field [13]. In order to not enforce

the algorithm to follow a given pathway, we consider that the initial trial field $E_0(t)$ is zero over a given duration T_0. The dependance of the final solution on the two parameters T_0 and α_0 will be analyzed in Sec. III C.

C. Numerical results

We first analyze the computational results for a system of two spins. Figure 1 displays the optimal solution computed by the algorithm for the values of parameters $T_0 = 0.5$ and $\alpha_0 = 0.08$. The parameter a which describes the evolution of the control duration at each step of the algorithm is taken to be 5×10^{-4}. Other values of a have been used leading either to worse results or to a slower convergence of the algorithm. As can be seen in Fig. 1, the evolution of the optimal control fields and of the probability is rather smooth with no rapid oscillation. A very good efficiency larger than 0.99 has been reached in 5000 iterations with a final duration of the order of $T = 2.035$. Note that a standard monotonically algorithm with this total duration leads to a solution very close to the ones obtained with this new algorithm. More precisely, for the standard algorithm, we have obtained a projection P larger than 0.999 for a control duration such that $1.9 < T < 2.4$. This computation shows that the time-optimal control algorithm has found the best compromise between the duration, the minimization of the distance to the target state and the energy of the field. As could be expected, the modification of the control duration slows down the convergence of the algorithm since a projection larger than 0.99 is obtained respectively after 2512 and 700 iterations for the new and standard methods, respectively. The monotonic behavior of the algorithm can be checked in Fig. 2 together with the evolution of the duration T_k. As for the cost J_k, one sees that this parameter presents a rapid increase for the first 3000 iterations and then an approximatively constant behavior. This means qualitatively that the time-optimal procedure first optimizes the control duration before decreasing the energy of the field without changing the total cost J. A crucial property that this algorithm must satisfy (at least locally) is the independence of the final solution with respect to the value of T_0, i.e. of the starting guess used to initiate the algorithm. This point is illustrated in Fig. 3 where two attraction points for the sequence (T_k) have been found when the time T_0 varies. We numerically determine the two basins of attraction and we found a boundary of the order of $T_0 \simeq 0.75$. Other attraction points exist for larger initial values of the control duration T_0

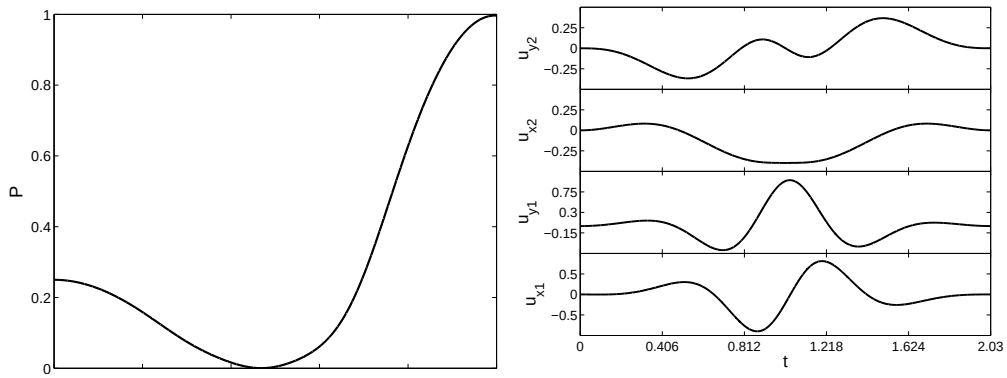

FIG. 1: Evolution of the probability P and of the corresponding optimal fields acting on the first or second spin. Numerical values are taken to be $\alpha_0 = 0.08$ and $T_0 = 0.5$. The final probability is $P = 0.9964$.

which are not represented in Fig. 3. Note that this attraction point characterizes not only the final control duration but also the final control fields and the final probability density as can been checked in Fig. 3. In Fig. 3, we see that a better efficiency is reached for $T_0 = 0.9$ with a longer and lower energetic optimal solution. This point indicates the importance of the control duration in the accuracy of the computation.

In Fig. 4, we study the evolution of the final time T_f and of the probability density P as a function of the parameter α_0. We observe that P increases and T_f decreases as the parameter α_0 decreases. As could be expected, the smaller α_0 is, the more energetic the optimal solution is since α_0 controls the relative weight of the pulse energy in the cost J. With a more energetic optimal solution, the algorithm can find an optimal solution with a lower duration and a better efficiency.

We extend these numerical results to the case of a four-spin system and a C^3NOT gate. Due to the complexity of this gate, a larger duration and a larger number of iterations are required to reach a sufficient efficiency. The parameter a is taken to be 5×10^{-4}. As for the two-spin case, we find two possible optimal solutions according to the value of T_0 which are displayed in Fig. 5. The time evolution of the probability density shows that the structure of these two solutions is very close even if the duration is different.

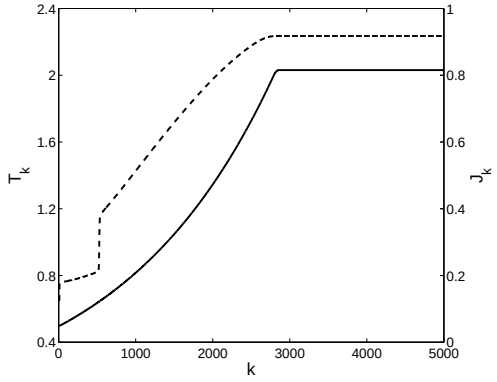

FIG. 2: Evolution of the cost J_k (dashed line) and of the time T_k (solid line) as a function of the number of iterations k of the algorithm. The same parameters (α_0 and T_0) as in Fig. 1 have been used.

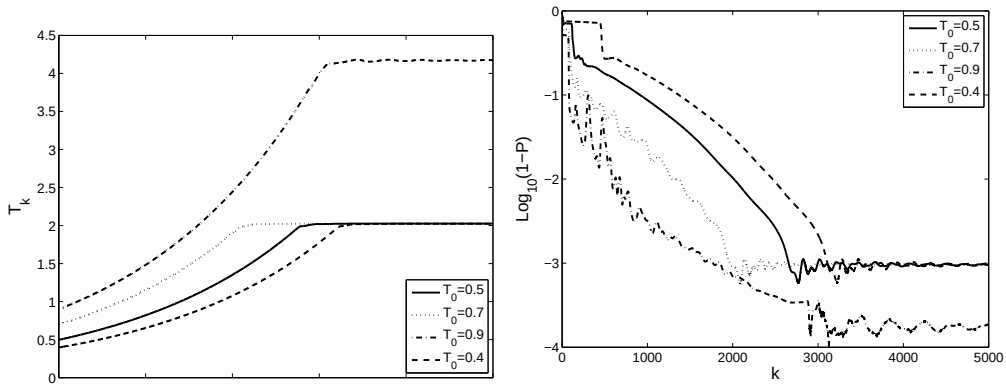

FIG. 3: (top) Evolution of the time T_k for different initial times T_0 as a function of the number k of iterations. For $T_0 \leq 0.7$, the algorithm converges towards the same optimal duration close to the value 2. The parameter α_0 is taken to be 0.08. (bottom) Same as before but for the probability density P. A better efficiency is reached for $T_0 = 0.9$.

IV. CONCLUSION AND PERSPECTIVES

This work deals with the time-optimal control of spin systems in NMR. We propose a monotonically convergent algorithm which both optimizes the control duration and the energy of the field. We show that the change of the duration at each iteration of the algorithm leads to a more flexible algorithm and thus allows a better convergence with respect to a standard version of such algorithms. This algorithm has the advantage of simplicity and general applicability whatever the quantum optimal control problem considered. We have

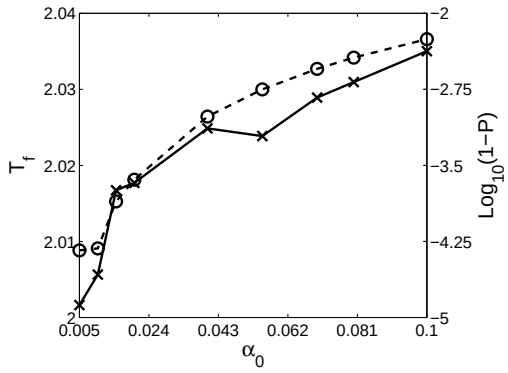

FIG. 4: Evolution of T_f (open circle) and P (cross) as a function of the parameter α_0 for $T_0 = 0.5$. The solid and dashed lines are just to guide the lecture.

finally demonstrated the possibility of implementing quantum gates from the control fields computed by this algorithm. Since there exists no unique optimal solution, we have shown that we can select the control fields by changing the initial control duration.

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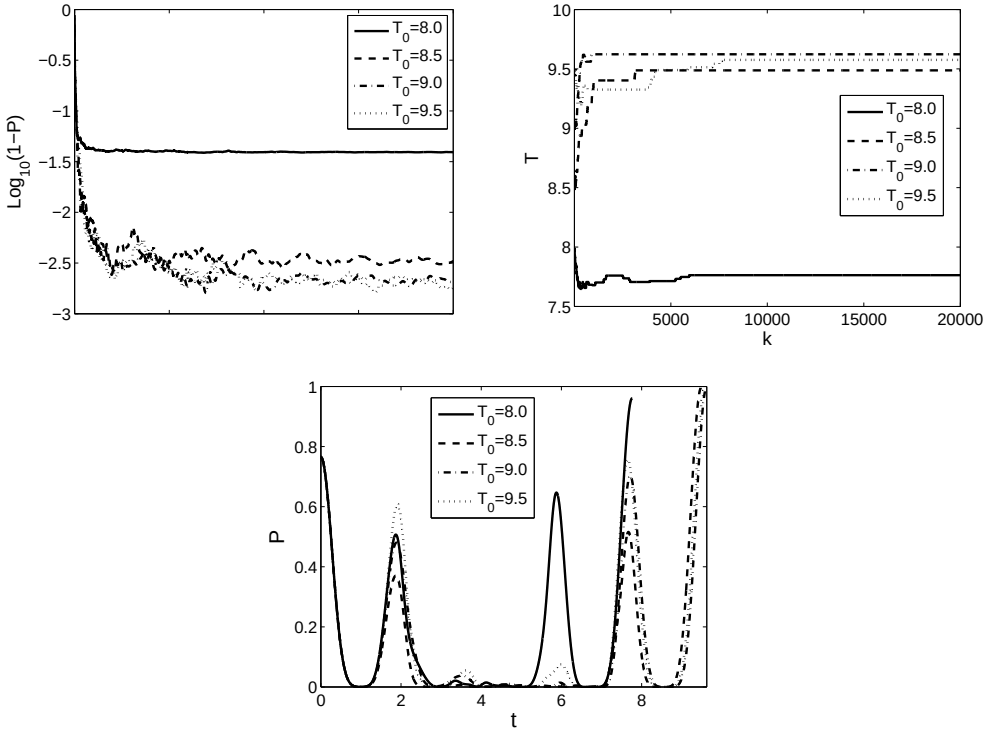

FIG. 5: (top-middle) Evolution of the probability density P and of the control duration T_k as a function of the number of iterations for different initial durations T_0. (bottom) Time-evolution of the probability density P for the different optimal solutions. The parameter α_0 is taken to be $\alpha_0 = 0.01$.

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