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Multiple Solutions in the Tracking Control of Quantum Systems†

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This paper demonstrates the existence of multiple solutions at each time point in tracking control of quantum systems. These solutions are shown to arise from the nonlinear dependence of the short-time propagators $U(t+\delta t,t)$ on the control field. The multiplicity of solutions depends on the parameters of the controlled system and the nature of the imposed track. Multiple solutions necessitate that a choice be made at each time point, resulting in an exponentially expanding space of distinct control fields that maintain the prescribed track. This behavior is illustrated by application to a small model system. The presence of multiple tracking control fields is consistent with behavior observed from quantum control landscape theory.

1. Introduction

The goal of tracking control is to find a field that induces an observable of a system to follow an a priori defined time-dependent track. Tracking control has been posed as a *local* optimization in time for applications to classical systems[1,2] and, recently, to quantum systems.[3−8] The technique differs from standard optimal control theory (OCT), which permits the observable to follow any path that achieves the given terminal value while satisfying the constraints or costs imposed on the field.[9−11] Tracking control is appealing because it permits the imposition of a physically motivated track and has the potential to avoid the computational expense of traditional global OCT calculations.

The concept of a quantum control landscape is relevant to understanding tracking and the success of quantum control experiments.[12−14] The quantum control landscape represents the mapping from the set of possible controls to the values of the control objective at a given dynamical time. The process of searching for an optimal control to accomplish a task at a given terminal time is an excursion across this landscape seeking to find a control solution that maps to the global optimum. It has been shown that the quantum control landscape is “trap-free”, having only global optima and possibly intermediate saddles, if the system is controllable and there are no significant constraints on the controls.[15] Furthermore, there are level sets of solutions at each objective value, including the global optimum.[7,16,17] Tracking control entails inverting an a priori track to identify one or more control fields ideally consistent with reaching the global optimum. For each time point along the track, there is a separate quantum control landscape. Each landscape, in isolation, may have a level set of solutions corresponding to the objective value at each time. Tracking control represents an excursion through this collection of quantum control landscapes. Despite the inherent trap-free nature of quantum control landscapes, the imposition of a track is a significant constraint on the allowed movement through these landscapes. Consequently, a solution may encounter a “false” trap forcing the observable value to deviate from the track. Nevertheless, tracking control creates the possibility that multiple routes through the collection of landscapes (each route representing a distinct control field) exist that can successfully follow the imposed track.

The theoretical justification for the invertibility of a track to identify a field in quantum control systems has been investigated,[18] and further work has developed practical tracking algorithms.[4−6,19] The possibility of multiple control fields able to follow prescribed tracks is explored in the present work. The multiplicity of control fields was raised in the related problem of inverting molecular dynamics tracking data to yield information about potentials.[20]

The structure of the paper is as follows: section 2 formulates the tracking problem and presents the origin of multiple solutions, section 3 illustrates this behavior through application to a simple model system, and conclusions are presented in section 4.

2. Formulation

Consider an N-level quantum system described by a field-free Hamiltonian, H_0, that interacts with an external control field, $\varepsilon(t)$, through a dipole, μ. The initial state of the system is described by the density matrix, ρ_0, which evolves under the influence of the control field in accordance with the equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = [H_0 - \mu\varepsilon(t), \rho(t)], \rho(0) = \rho_0 \tag{1}$$

where [,] is the operator commutator. The observable is represented by the Hermitian operator O, whose expectation value at time t is given by $\langle O\rangle_t = Tr[\rho(t)O]$. The prescribed track for the expectation value is given by $f(t)$, for $t \in [0,T]$. To rigorously maintain the track, the following condition must be satisfied:

$$Tr[\rho(t)O] = f(t), 0 \le t \le T \tag{2}$$

One approach to tracking[5] is based on differentiating eq 2 to yield

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$$\frac{df(t)}{dt} = \frac{d[Tr(\rho O)]}{dt} = \frac{Tr([H_0 - \mu\varepsilon(t), \rho(t)]O)}{i\hbar} \quad (3)$$

The procedure is to solve for $\varepsilon(t)$ on the right-hand side with $df(t)/dt$ known from the prescribed track $f(t)$. This equation is highly nonlinear in $\varepsilon(t)$ through the implicit dependence of $\rho(t)$ on the field. A common technique is to use the explicit dependence on $\varepsilon(t)$ in the right-hand side of eq 3 to get a single local solution. Below, we examine the true nonlinear nature of the tracking problem.

It is convenient to discretize the time dependence in steps of δt to explore the nonlinear dependence of eq 3 on $\varepsilon(t)$. This renders the control field, $\varepsilon(t)$, a piecewise constant function of time. This is done so that the Hamiltonian, $H(t) = H_0 - \mu\varepsilon(t)$, may be treated as independent of time over each short time interval δt. Under this condition, eq 1 yields the following expression for $\rho(t+\delta t)$

$$\rho(t + \delta t) = U(t + \delta t, t)\, \rho(t)\, U^{\dagger}(t + \delta t, t) \quad (4)$$

where

$$U(t + \delta t, t) = \exp[-i(H_0 - \mu\varepsilon(t))\delta t/\hbar] \quad (5)$$

is the short-time propagator with $\varepsilon(t)$ treated as constant over the interval $[t, t + \delta t]$. From eq 2, the necessary condition on the field to maintain the track over $t \rightarrow t + \delta t$ is

$$f(t + \delta t) = Tr[U(t + \delta t, t)\, \rho(t)\, U^{\dagger}(t + \delta t, t)O] \quad (6)$$

which is a nonlinear function of $\varepsilon(t)$ in the current time step, through $U(t+\delta t,t)$. A root of eq 6 is a field value, $\varepsilon(t)$, that maintains the track for the observable at time $t + \delta t$. The roots can be found by a line search over eq 6. In some cases, the imposed tracking step $t \rightarrow t + \delta t$ results in a singularity, defined as there being no roots to eq 6. However, given the oscillatory dependence of $U(t+\delta t,t)$ on $\varepsilon(t)$, the expectation is that a large number, perhaps even an infinite number, of roots may exist. A variant of tracking is to ask that $\langle O \rangle_t$ increase (or decrease) over time rather than follow a specific track.[21] In this case, eq 6 becomes $f(t+\delta t) - f(t) > 0$. Although this inequality criterion is less demanding than eq 6, trapping of the observable value along any particular path $\varepsilon(0) \rightarrow \varepsilon(\delta t) \rightarrow \varepsilon(2\delta t)$ etc. may still occur.

From eq 5, it is evident that the short time propagator, $U(t+\delta t,t)$, depends on the operators (H_0 and μ), the time step (δt), and the current field amplitude [$\varepsilon(t)$]. The propagator $U(t+\delta t,t)$ is parametrized by the field amplitude $\varepsilon(t)$, and a toolkit of short-time propagators, $\Omega_l = \exp[-i(H_0 - \mu\varepsilon_l)\delta t/\hbar]$, can be generated by sampling field values ε_l ($l = 1, 2,..., L$), at a desired resolution within some bounds. The members of the toolkit Ω_l can then be searched over to find the roots to eq 6, within the resolution of the toolkit. This search procedure is repeated at each time step with the same toolkit. By sequentially searching over field values and picking a particular root of eq 6 at each time step, a control field, $\varepsilon(n\delta t)$ for $n = 0, 1, 2, 3,...$, can be constructed that forces the observable to follow the imposed track. The number of roots at each time point is dependent on the current state of the system and the system Hamiltonian.

This procedure can only be followed if eq 6 has at least one root at each time step. The absence of a root would indicate a singularity and a necessary deviation from the track in order to make further progress. In this case, one may also take a step backward (i.e., backtrack) in time and choose another prior root. The multiplicity of roots at each time point creates an exponential explosion in the number of possible fields while proceeding along the track. It is not possible to a priori discover the right root at each time that would allow the system to continue to adhere to the track out to the final time T.

3. Illustrations

The identification of multiple solutions was observed in various simulations, and for initial illustration, we consider a simple three-level system

$$H_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 9 \end{pmatrix} \quad \mu = \begin{pmatrix} 0 & 1.457 & 2.3805 \\ 1.457 & 0 & 2.2162 \\ 2.3805 & 2.2162 & 0 \end{pmatrix} \quad (7)$$

The system is initially in the ground state, $|\psi(0)\rangle = |1\rangle$, and the observable is $O = |3\rangle\langle 3|$, corresponding to the goal of tracking the transition probability of $|1\rangle \rightarrow |3\rangle$. For simplicity, we choose a linear track, $f(t) = 0.5t$ for $t \geq 0$, to illustrate the qualitative tracking features, although the same behavior should be observed for an arbitrary track. Given these parameters, the density matrix becomes $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ with $|\psi(t)\rangle = U(t,0)|\psi(0)\rangle$ being the state. Equation 6 reduces to

$$f(t + \delta t) = |\langle 3|U(t + \delta t, t)|\psi(t)\rangle|^2 \quad (8)$$

and results will be shown for 10 time steps of size $\delta t = 0.1111$ out to $T = 1.0$. The propagator toolkit was generated by sampling field amplitudes in the range $[-20,20]$ at a resolution of 0.001. However, for the purpose of illustrating the algorithm it is sufficient to seek roots over a limited amplitude range taken as $[-5,5]$.

At $t = 0$, there is only a single root at $\varepsilon(0) = 0$ in the domain $\varepsilon \in [-5,5]$. Generally, however, nonzero values for $\varepsilon(0)$ could exist, still giving the initial track value $f(0) = 0$ (e.g., such roots do exist for this case outside of the domain $\varepsilon \in [-5,5]$, as evident in Figure 1a). Having chosen the initial value, the roots at the two subsequent time steps are shown in Figure 1 (the plots include field values outside of the domain $[-5,5]$). The values of subsequent possible roots depend on the choice of roots at each of the previous time steps, since these choices define the successful evolving control field and the nature of the current state of the system. For example, choosing root A in Figure 1a leaves the system in the state $|\psi_A(\delta t)\rangle = U(\delta t,0)|1\rangle$, where the propagator $U(\delta t,0)$ implicitly depends on the choice of field amplitude (cf., eq 5). At the subsequent time, $t = 2\delta t$, the field amplitude is selected from the points of intersection of the track $f(2\delta t)$ and the transition probability $|\langle 3|U(2\delta t,\delta t)|\psi_A(\delta t)\rangle|^2$, as shown in Figure 1b. There is a similar progression from part a to part b of Figure 1 on choosing root B. Exhaustive exploration of all possible solutions (i.e., tracing the rapidly growing number of distinct fields over time) is only possible over a small number of time steps.

The fields have distinct characteristics, and a small selection is shown in Figure 2. The effects of the chosen track and imposed limits on field amplitude can be understood from Figure 1. For example, if the track had demanded that, say $f(t{=}2\delta t) = 0.03$, then no roots would have been found within the search region $[-5,5]$ of field amplitudes in Figure 1. However, roots can be found over the extended range of $\varepsilon_l \in [-20,20]$. Depending on the choice of roots over the progression of the

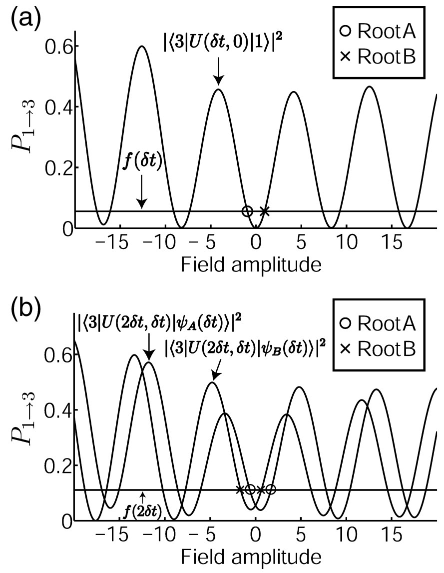

Figure 1. The oscillatory curves are $P_{1\to3} = |\langle 3|U(n\delta t,0)|1\rangle|^2$ as a function of ε from the right-hand side of eq 8 with (a) $n = 1$ and (b) $n = 2$. The horizontal lines are the left-hand side of eq 8. For illustration, the root search is confined over the interval [−5,5] in the field amplitude, although roots exist outside of this interval. In part a, choosing root A leaves the system in the state $|\psi_A(\delta t)\rangle$ at $t = \delta t$, which leads to the oscillatory function $|\langle 3|U(2\delta t,\delta t)|\psi_A(\delta t)\rangle|^2$ at $t = 2\delta t$ in part b. Similarly, choosing root B in part a leaves the system in the state $|\psi_B(\delta t)\rangle$ at $t = \delta t$, which leads to the oscillatory function $|\langle 3|U(2\delta t,\delta t)|\psi_B(\delta t)\rangle|^2$ at $t = 2\delta t$ in part b. Accordingly, in part b both cases A and B have two possible roots for $\varepsilon(2\delta t)$. For later times, this behavior leads to a rapidly increasing, nearly exponential, number of roots, although some paths lead to singularities.

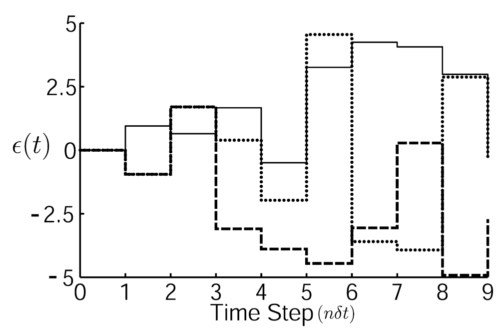

Figure 2. A small subset of fields are shown that exactly follow the track. It is evident that the solution fields encompass a diverse range of forms.

tracking algorithm, either family of evolving roots A or B in Figure 1 could hit a singularity at a subsequent time step.

From the study of a variety of systems, generally there is an observed exponential growth of roots early in the tracking process, i.e., each root at time $n\delta t$ gives rise to M additional roots at time $(n + 1)\delta t$. As the tracking procedure progresses, the observed exponential growth is retarded as a number of subsequent roots falls outside the search region and as a subset of root choices leads to singularities. As an illustration, Figure 3 shows the number $\mathcal{N}$ of control fields achieving the track through time $t = n\delta t$ over a representative run of the algorithm. There is an exponential increase in the number of fields meeting the track over time for $n = 0,..., 4$, where the growth rate is $M \approx 4$. The origin of the rapid rise in roots is already evident in the example shown in Figure 1, where the growth rate is $M \approx 2$, i.e., two roots grow to four in the second time step. The example in Figure 3 also shows that singularities increase over time for $n = 5,..., 9$ slowing the exponential growth of control solutions. This growth in singularities reduces the number of fields successfully meeting the track as they are removed at each time step.

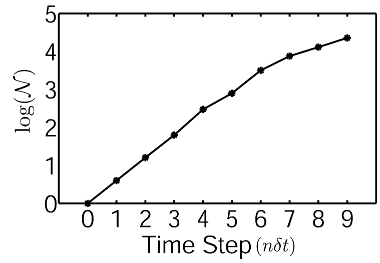

Figure 3. Number $\mathcal{N}$ of control fields that meet the desired track through $t = n\delta t$. Early in the tracking process, $n = 0,..., 4$, the number of acceptable fields increases nearly exponentially. As the procedure continues, roots begin to fall outside of the search region and the number of fields that encounter singularities increases, thereby slowing the exponential growth.

Various relaxed forms of tracking may also be considered to lessen the strict demand of exactly following an imposed track over time. In this regard, one reasonable cost function J seeking to maximize $\langle O(t)\rangle$ while minimizing the local field amplitude is $J[\varepsilon(t)] = \langle O\rangle_t^2 - \omega[\varepsilon(t)]^2$, where $\omega > 0$ is a weight factor. The roots for this formulation of the problem can be found in the same fashion as for eq 8 using the propagator toolkit. This procedure produces results (not shown here) that are analogous to the exact tracking case illustrated in Figure 1. As with the local tracking procedure, field trapping can also occur for relaxed tracking depending on the choice of ω and the structure of the Hamiltonian.

4. Conclusion

This paper demonstrates that multiple solutions exist to quantum mechanical tracking control. These solutions arise from the nonlinear and oscillatory nature of the tracking control equation (cf., eq 2) with respect to the field amplitudes. Multiple piecewise constant control solutions can be found through a simple search process over a propagator toolkit at each time point. However, there is always the possibility that the search may encounter a singularity with no field amplitude existing in the search interval that meets the imposed track. In these cases, an iterative procedure of backtracking may be employed, but that will increase the computational expense of achieving tracking control. Nevertheless, tracking control still has attractive features associated with its simple formulation.

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