Quantum Wave Function Controllability

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Abstract

Theoretical results are presented on the ability to arbitrarily steer about a wavefunction for a quantum system under time-dependent external field control. Criteria on the field free Hamiltonian and the field coupling term in the Hamiltonian are presented that assure full wavefunction controllability. Numerical simulations are given to illustrate the criteria. A discussion on the theoretical and practical relationship between dynamical conservation laws and controllability is also included.

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1 Introduction

There is much interest on controlling quantum systems through their interaction with external fields [1] - [11]. This activity is motivated by a potential wide range of applications [7] that this framework can accommodate. Encouraging positive results have already been obtained in closed loop experiments [12, 13], but both theoretical and experimental research is still needed to understand the subtle nature of the control processes.

Early efforts at achieving quantum control based on intuitive physical understanding generally gave poor results. Significant advances have come through the introduction of rigorous control theory tools together with enhanced laser pulse shaping capabilities. An important preliminary step to any experiment are indications of its feasibility through theoretical studies and computer simulations. Such analyses can indicate the set of objectives that can reasonably be met and present the nature of a laser pulse to most likely meet the objectives. The study of the set of quantum states that can

be attained is an aspect of control theory aimed at deciding whether the system is *controllable*, i.e. if any admissible quantum state can be attained with some (admissible) laser field. Until recently the answer to this question was given using results available in [14] or [15] ; although useful in many cases, these results may prove more general than often required, as in [14] where general results are derived for the evolution of unitary operators, or too pessimistic as in [15] where negative results are presented for infinite dimensional controllability. A theoretical study was then undertaken [16] to shed some light on the phenomena involved when controllability for the wavefunction is investigated in finite dimensional bilinear quantum systems. The purpose of this paper is to explore and discuss the practical utility of these latter formal theoretical results along with simple illustrations through computer simulations. The outline of the paper is as follows: the theoretical results are presented in section 2 ; supporting numerical simulations and some practical extensions of the theory are presented in section 3. A discussion on the connections between dynamical conservation laws and controllability of quantum systems is given in section 4 ; concluding remarks are presented in section 5.

2 Theoretical Controllability Criteria

Consider a quantum system with internal Hamiltonian H_0 prepared in the initial state $\Psi_0(x)$, where x denotes the relevant coordinate variables. The external interaction will be taken here as a control field amplitude $\epsilon(t) \in \mathbb{R}$ coupled to the system through a time independent (e.g, dipole moment) operator $\mathcal{B}$ (see also [17]) ; then the time-dependent control Schrödinger equation that gives the evolution of the state $\Psi(x,t)$ at time t is :

$$\begin{aligned} i\hbar\tfrac{\partial}{\partial t}\Psi(x,t) = &\quad H_0\Psi(x,t) + \epsilon(t)\cdot\mathcal{B}\Psi(x,t) = H\Psi(x,t) \\ \Psi(x,t=0) = &\quad \Psi_0(x) \end{aligned} \tag{1}$$

In order to avoid trivial control problems we suppose $[H_0, \mathcal{B}] \neq 0$, where the Lie bracket $[\cdot,\cdot]$ is defined as $[U,V] = UV - VU$.

The goal is to find if any final time $T > 0$ and finite energy control pulse $\epsilon(t) \in L^2([0,T])$ exist such that $\epsilon(t)$ is able to steer the system from $\Psi_0(x)$ to some predefined target $\Psi(x,T) = \Psi_{target}(x)$. If the answer to this question is affirmative, then the system is controllable. Given that H is Hermitian, the L^2 norm $\|\Psi(x,t)\|_{L^2_x(\mathbb{R}^\gamma)}$ of Ψ is conserved throughout the evolution so that $\Psi(x,t)$ evolves on the unit sphere $S(0,1)$ of $L^2(\mathbb{R}^\gamma)$:

$$S(0,1) = \{f \in L^2(\mathbb{R}^\gamma); \|f\|_{L^2(\mathbb{R}^\gamma)} = 1\}$$

Numerical simulations on the system (1) require the introduction of a finite dimensional setting. A common choice is to consider the set $D = \{\Psi_i(x); i = 1, .., N\}$ of the first N eigenstates of the infinite dimensional Hamiltonian H_0 and restrict the operators involved to the linear space that D generates. Let A and B be the matrices of the operators H_0 and $\mathcal{B}$ respectively, in terms of this base, and as above, it is supposed that $[A, B] \neq 0$.

Before leaving the infinite dimensional setting, we remark that the controllability of (bilinear) quantum systems on infinite dimensional spaces is a difficult problem and the resolution of this matter is only partially solved. Moreover, the generic results obtained so far in this setting are **negative** [20, 15, 21, 22, 23] showing the need for tailored controllability concepts and a thorough understanding of the finite dimensional case in order to appropriately extend the **positive** controllability results available [14, 16] to the infinite dimensional setting. The present study is also motivated by the existence of intrinsically finite dimensional quantum mechanical situations (e.g. N-level spin systems, etc.).

We denote $C = (C_i)_{i=1}^N$ to be the coefficients of $\Psi_i(x)$ in an expansion of the evolving state $\Psi(t, x) = \sum_{i=1}^N C_i(t)\Psi_i(x)$, $N \geq 3$; Eq (1) now becomes

$$\begin{cases} i\hbar\frac{\partial}{\partial t}C = AC + \epsilon(t)BC \\ C(t=0) = C_0 \end{cases} \tag{2}$$

$$C_0 = (C_{0i})_{i=1}^N,\ C_{0i} =< \Psi_0, \Psi_i >,\ \sum_{i=1}^N |C_{0i}|^2 = 1 \tag{3}$$

The controllability of Eq. (2) has been already dealt with in the literature [14] by considering the problem of the controllability of a system posed on the space of the unitary matrices of dimension N. This elegant approach has the benefit of drawing on the general tools and results from bilinear controllability on Lie groups. However, verifying those criteria may be computationally difficult when N is large; moreover the results obtained this way give only sufficient conditions for exact controllability (due to a setting that is more general than often required). Thus, we consider identifying computationally convenient and intuitive conditions for finite dimensional wavefunctions to be reachable from an arbitrary initial state (see also [24] for an overview of the topic).

We make the common assumptions that the A matrix is diagonal and that the B matrix is real symmetric (Hermitian). Denote $\lambda_i \in \mathbb{R},\ i = 1, .., N$, as the real diagonal elements of A (i.e. the energies associated with the states Ψ_i). Denote $S_M(0, 1) = S(0, 1) \cap M$. The conservation of the L^2 norm of the wavefunction can be written in the finite dimensional representation:

$$\sum_{i=1}^{N} |C_i(t)|^2 = 1, \ \forall t \geq 0 \tag{4}$$

2.1 Connectivity Graph

The B matrix plays the critical role of specifying the kinematic coupling amongst the eigenstates of the system reference Hamiltonian matrix A. The structure of the set of all direct and indirect couplings between eigenstates is very relevant to assessing controllability. In order to formalize the concepts, we associate to the system a non-oriented graph $G = (V, E)$ called the *connectivity graph* (the reader is referred to [25] for graph theory concepts). We define the set V of vertices as consisting of the eigenstates Ψ_i and the set of edges E as consisting of all pairs of eigenstates **directly** coupled by the matrix B.

$$G = (V, E): \quad V = \{\Psi_1, ..., \Psi_n\}, \quad E = \{(\Psi_i, \Psi_j); i < j, \ B_{ij} \neq 0\} \tag{5}$$

This graph can be decomposed into (connected) components $G_\alpha = (V_\alpha, E_\alpha)$, $a = 1, .., K$. In more intuitive terms, two eigenstates Ψ_α and $\Psi_{\alpha'}$ are in the same connected component (we will say that they are *indirectly coupled*) if there exist a path $\Psi_{j_1} = \Psi_\alpha$, Ψ_{j_2},..., $\Psi_{j_l} = \Psi_{\alpha'}$ from Ψ_α to $\Psi_{\alpha'}$ such that any **consecutive** vertices Ψ_{j_a} to $\Psi_{j_{a+1}}$ of this chain are *directly coupled*, i.e. the dipole moment $B_{j_a j_{a+1}}$ is non-zero (which is the same as $(\Psi_{j_a}, \Psi_{j_{a+1}}) \in E$) ; note that there is no need for non-consecutive vertices Ψ_{j_a} to Ψ_{j_b} to be directly connected, i.e. if $b \neq a+1$ and $a \neq b+1$ the entry $B_{j_a j_b}$ may be zero. This decomposition corresponds to a bloc-diagonal structure of the matrix B (modulo some permutations on the indices), so it is just a matter of specifying the number of independent subsystems we want to **simultaneously** control (see [21] for the general case). We will consider the following hypothesis as true

$\mathbb{HA}$ *The graph G is connected, i.e. $K = 1$.*

Remark 1 *In agreement with the definition above, note that $\mathbb{HA}$ does* **not** *imply that any two states are necessarily* **directly** *connected, one with the other, but only that for any two states Ψ_α and $\Psi_{\alpha'}$ there is a path in the graph G that connects Ψ_α and $\Psi_{\alpha'}$.*

Denote by $U(A, B, \epsilon, t_1 \to t_2)$ the propagator associated with Eq. (2); for any state $\chi(t_1)$, $U(A, B, \epsilon, t_1 \to t_2)\chi(t_1)$ is defined as the solution at time $t = t_2$ of Eq. (2) with the initial state at time $t = t_1$ being $\chi(t_1)$.

Definition 1 *We say that* $\tilde{\Psi}$ *is reachable from* $\overline{\Psi}$ *if there exists* $0 < T < \infty$, $\epsilon(t) \in L^2([0,T];\mathbb{R})$ *such that* $U(A,B,\epsilon(t),0 \to T)\tilde{\Psi} = \overline{\Psi}$.

2.2 Controllability

Denote $\omega_{kl} = \lambda_k - \lambda_l,\ k,l = 1,...,N$ as the eigenvalue differences for the matrix A, and atomic units ($\hbar = 1$) will be utilized. Consider the hypothesis:

$\mathbb{HB}$ *The graph* G *does not have "degenerate transitions", that is for all* $(i,j) \neq (a,b)$, $i \neq j$, $a \neq b$ *such that* $B_{ij} \neq 0$, $B_{ab} \neq 0$*:* $\omega_{ij} \neq \omega_{ab}$.

Remark 2 *This hypothesis could be relaxed to requiring only that the graph* G *remains connected after elimination of all edge pairs* $(\Psi_i,\Psi_j),(\Psi_a,\Psi_b)$ *such that* $\omega_{ij} = \omega_{ab}$ *(degenerate transitions). However, to ease of presentation,* $\mathbb{HB}$ *will be assumed to be true.*

We also introduce one more hypothesis:

$\mathbb{HC}$ *For each* $i,j,a,b = 1,...,N$ *such that* $\omega_{ij} \neq 0$*:* $\frac{\omega_{ab}}{\omega_{ij}} \in Q$, *where* Q *is the set of all rational numbers.*

Remark 3 *Alternative controllability results completely excluding the need of the assumption* $\mathbb{HC}$ *are also possible and will be presented in a future paper.*

The main controllability result in [16] can be summarized as follows:

Theorem 1 *Under the assumptions* $\mathbb{HA}$, $\mathbb{HB}$, $\mathbb{HC}$ *the system (2) is controllable, that is for any* $\Psi \in S_M(0,1)$ *the set of reachable states from* Ψ *is* $S_M(0,1)$.

Remark 4 *Under the assumption* $\mathbb{HB}$, *the controllability criteria above has very strong uniform properties with respect to the coupling matrix* B. *Indeed, the only information needed to know is whether* B_{ij} *is null or not for each* $i,j = 1,...,N$ *; the* **exact value** *of* B_{ij} *is not important. Thus, the controllability analysis is generally independent of small errors in the entries of* B. *Note also that when adding, for example, one more eigenstate to the basis* D, *the controllability criterion is easy to check for the new system: it is necessary to ensure that the new state is connected through* B *to at least one eigenstate in the old basis and then check that the transition energies thus introduced do not equal other transition energies in the system - non-degeneracy - (see also remark 2).*

When $\mathbb{HB}$ is not satisfied, changing the exact values of the entries of the coupling matrix B may transform a system that is not controllable into a system that is controllable; other techniques that allow for assessing the controllability (see the situation presented in Eq. (7) later in section 3) may also be sensitive to changes in coupling matrix entries.

Remark 5 *Theorem 1 is a result complementary to the work in [14] as the settings are different. Thorem 4.2 in [14] is appropriate when controllability on spaces of unitary matrices is under study (e.g., in quantum computing and in general where the Lie group transformation structure is relevant to the system), while theorem 1 above is suitable for assessing wavefunction controllability. Extensions of theorem 1 are available in [21] for the case of multiple independent subsystems (non connected graphs) along the same paradigm.*

A detailed proof of theorem 1 may be found in [16]. Below we go beyond the latter work and demonstrate the physical meaning and applicability of the theorem.

3 Numerical Simulations

Numerical experiments have been undertaken to illustrate the theoretical result above. All of the examples correspond to model systems with an external laser electric field coupled in through a dipole matrix B. The controllability Theorem 1 is not constructive in that its satisfaction does not produce a particular control field. Thus the controlling fields in the examples were computed using a genetic algorithm search procedure. Consider the following model [26] five-level system having internal Hamiltonian and coupling matrices,

$$A = \begin{pmatrix} 1.0 & 0 & 0 & 0 & 0 \\ 0 & 1.2 & 0 & 0 & 0 \\ 0 & 0 & 1.3 & 0 & 0 \\ 0 & 0 & 0 & 2.0 & 0 \\ 0 & 0 & 0 & 0 & 2.15 \end{pmatrix}, \; B = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{pmatrix}. \tag{6}$$

Prior numerical studies with optimal control calculations hinted that this system might be controllable, but such computations cannot assure a full assessment (c.f., discussion later in this section). The coupling graph of the system plotted in Figure 1 is obviously connected. In addition, it can be easily checked that the system has non-degenerate transitions. It follows by the controllability theorem that this system is completely controllable,

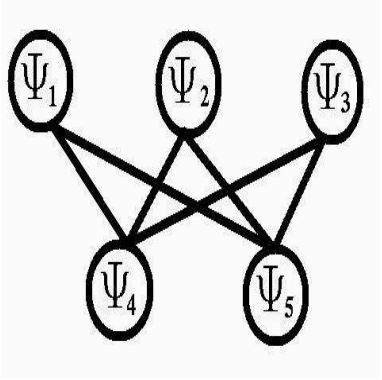

Figure 1: The graph associated with the B matrix of the system in (6). Note that the graph remains connected even after removal of some edges, e.g., (Ψ_3, Ψ_4) and (Ψ_1, Ψ_5).

implying that any superposition of states is reachable from any other in finite time and with finite laser energy.

An example of control is given in Figure 2; we plot the overlap of the wavefunction with the initial state and the distance to the target state. This situation was choosen to demonstrate control to a superposition of states. The initial state was taken to be Ψ_4 and the target was set to $\frac{\sqrt{3}}{3}\Psi_1 + \frac{\sqrt{6}}{3}\Psi_2$. The target goal is achieved to high accuracy at $T_{final} = 550$.

Although theorem 1 is true only with satisfaction of the hypothesis $\mathbb{HB}$, various situations where $\mathbb{HB}$ at first glance appears to be violated may arise in practice. In this case a simple technique is available to assess if $\mathbb{HB}$ is valid and then return to the setting that accommodates theorem 1. One such example is given below.

Consider the system given by the following Hamiltonian and dipole moment matrix [27, 28]:

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & .004556 & 0 & 0 \\ 0 & 0 & 0.095683 & 0 \\ 0 & 0 & 0 & 0.095683 \end{pmatrix}, \; B = \begin{pmatrix} 0 & 1 & 1 & -1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix}. \quad (7)$$

As presented, the system does not comply with $\mathbb{HB}$, being degenerate $\lambda_3 = \lambda_4 = 0.095683 E_h$ and therefore with degenerate transitions e.g. $\lambda_3 - \lambda_1 = \lambda_4 - \lambda_1$. However the states 3 and 4 can be distinguished by having different dipole moments with state 1, and therefore the system is expected to be controllable, as suggested by numerical optimal control calculations [27, 28].

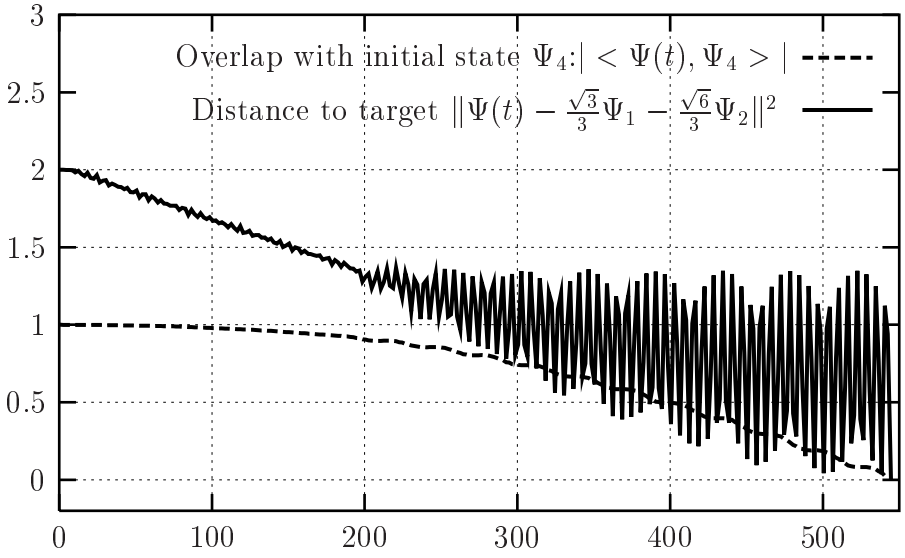

Figure 2: The evolution of the system in (6) under a control field realizing the target: $\Psi(T_{final}) = \frac{\sqrt{3}}{3}\Psi_1 + \frac{\sqrt{6}}{3}\Psi_2$.

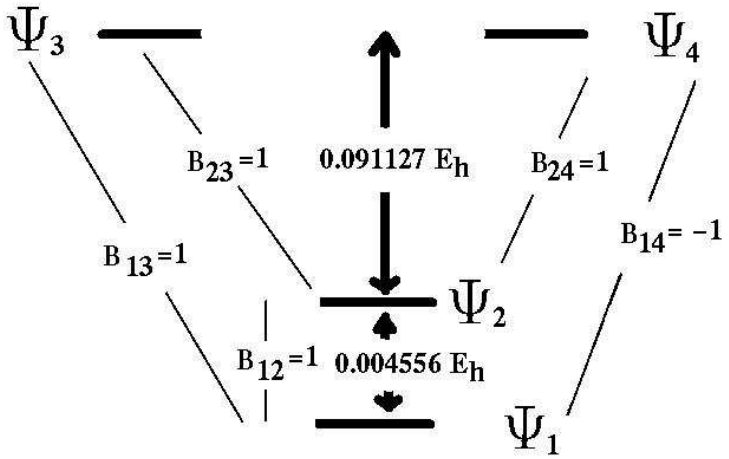

Figure 3: Graphical representation of the system in Eq. (7). It is seen that energy level degeneracy is present.

Note that by writing $\epsilon(t) = \mu + \tilde{\epsilon}(t)$ the triplet $(A, B, \epsilon(t))$ that characterizes the control system is transformed to $(A + \mu B, B, \tilde{\epsilon}(t))$. Here $A + \mu B$ is the matrix of the new Hamiltonian $H_\mu = H_0 + \mu\mathcal{B}$. A unitary matrix U_μ may be found such that $\tilde{A} = U_\mu(A + \mu B)U_\mu^t$ is diagonal, and the dipole matrix B changes accordingly $\tilde{B} = U_\mu B U_\mu^t$. The dynamical equations to control are now

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\tilde{C} = \tilde{A}\tilde{C} + \tilde{\epsilon}(t)\tilde{B}\tilde{C} \\ \tilde{C}(t=0) = U_\mu C_0 \end{cases} \tag{8}$$

It can be proven (and it is also trivial to check as soon as the precise value of μ is known) that the number of connected components of the connectivity graph $\tilde{G}$ associated to $\tilde{B}$ is the same as the connected components of G and so, according to hypothesis $\mathbb{HA}$, $\tilde{G}$ is connected. Therefore if $\tilde{A}$ complies with $\mathbb{HB}$ it follows (see also the remark 3) that the system under study is controllable. The controllability of the initial system (2) reduces then to finding μ such that $A + \mu B$ has no degenerate transitions. Many values for μ are often acceptable. The constant μ may be viewed as a Stark field which acts to suitably shift the energy levels so as to remove the degenerate transitions. However, this procedure is just a mathematical construction to reveal if the criteria underlying theorem 1 are valid. The identification of $\mu \neq 0$ does not imply that a laboratory implementation of the control requires a DC bias field to be successful. Satisfaction of $\mathbb{HA}$, $\mathbb{HB}$, $\mathbb{HC}$ just assure that at least some control exists to steer about the system in any arbitrary manner. As an illustration of the procedure above consider the example in Eq. (7) with $\mu = 0.1$ and then the eigenvalues of $A + \mu \cdot B$ are -0.172362, -0.042466, 0.170297 and 0.240453 (non-degenerate). It is easy to check that the eigenvalues also comply with $\mathbb{HB}$. The system (7) is therefore completely controllable. So, despite the degeneracy in the Hamiltonian, it is possible for instance to steer the system from from the state $\Psi(0) = \Psi_1$ to $\Psi(T) = \Psi_4$; such a laser pulse is presented in Figure 4 together with the evolution of the populations of the eigenstates in Figure 5.

In practice, the design of a control is implemented by the computation of a laser pulse that best meets the prescribed goals ; a general approach to executing this search is through the formalism of optimal control theory (OCT) where a cost functional for optimization is constructed that contains penalties for missing the target and various other costs (e.g. the fluence of the laser). A simple choice for such a cost functional is :

$$J(\epsilon, T) = \|\Psi_\epsilon(T) - \Psi_{target}\|^2 + \alpha \int_0^T \epsilon^2(t)dt \tag{9}$$

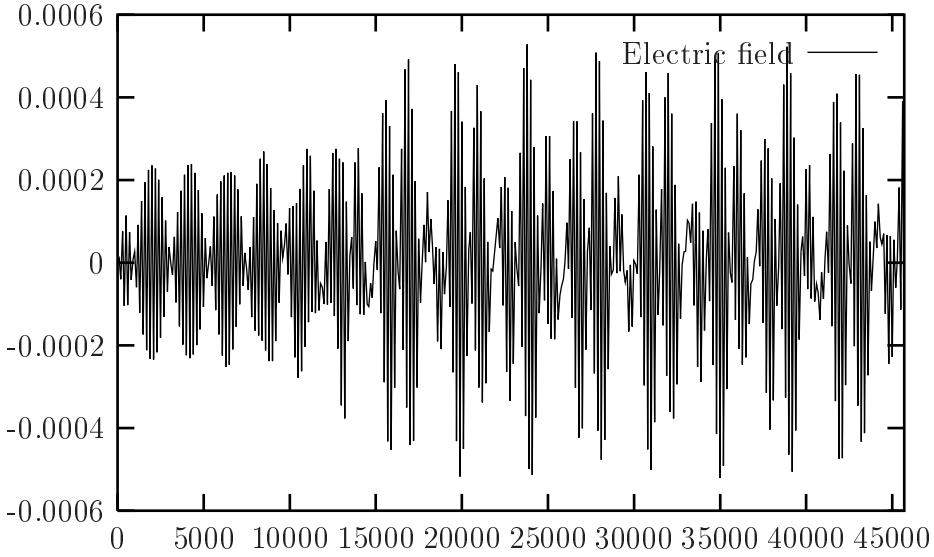

Figure 4: The field realizing the target $\Psi(T_{final}) = \Psi_4$ for the system in (7).

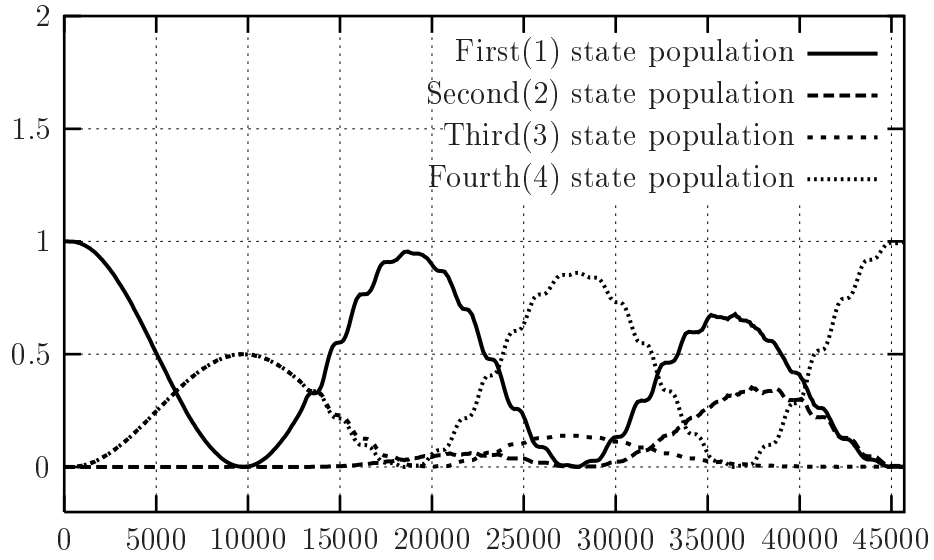

Figure 5: Evolution for the system (7) and field in Figure 4.

It is important to stress that theorem 1 (as any other **exact** controllability theorem) does not guarantee quantitative results for the minimization of $J(\epsilon, T)$, but only insures that in the absence of costs beyond reaching the target state (e.g., the fluence term in Eq. (9)) the minimum value of $J = 0$ **can** be reached for some $T > 0$ and $\epsilon_0(t) \in L^2([0, T])$. An analysis of the existence of at least one minimiser to a class of quantum mechanical OCT cost functionals is given in [6]. The trade-off between the two extremes of fully reaching the target state versus fully meeting the additional cost criteria is the task of the OCT optimization. In this framework, any field that gives exact controllability is a minimizer of $J(\epsilon, T)$ for $\alpha = 0$. When other values for α are chosen, the fluence generally will be smaller but the overlap with the the target will also be reduced. In the example of Figures 4 and 5 where the target was required to be exactly reached, the laser fluence was 0.0302. In another example (not shown here) the fluence term was retained in the OCT cost functional and an overlap with the target of 80% was achived. The optimal field was found to reduce the fluence to 0.021 at the expense of dropping the yield in the target state.

4 Dynamical Conservation Laws and Controllability Restrictions

In light of the manipulations on the system in Eq. (7) an Figure 3 it may seem that the hypothesis $\mathbb{HB}$ has merely a technical role. Therefore a legitimate question to ask is whether theorem 1 remains true in the absence of this assumption. The answer to this question is negative and the presentation of some very particular phenomena that arise when $\mathbb{HB}$ is invalid is the purpose of this section.

We begin with some simple observations. For any Hermitian operator O such that the commutators $[H_0, O]$ and $[\mathcal{B}, O]$ are both zero it is easy to prove that :

$$< \Psi(t)|O|\Psi(t) >=< \Psi_0|O|\Psi_0 >, \ \forall t > 0. \tag{10}$$

The quantity $< \Psi(t)|O|\Psi(t) >$ is therefore **conserved** during the evolution of the system, irrespective of the field $\epsilon(t)$. The presence of any conservation relation on $\Psi(t)$, other than Eq. (4), implies some controllability restrictions.

One special class of Hermitian operators are L^2-projections to closed subspaces. Let P be such a projection to a closed subspace X of $L^2(\mathbb{R}^\gamma)$. The equalities $[H_0, P] = [\mathcal{B}, P] = 0$ mean in particular that X and its orthogonal

complement $X^{\perp}$ are involutive for H_0 and $\mathcal{B}$, i.e.

$$\begin{cases} \forall \Psi \in X: \ H_0 \Psi \in X, \ \mathcal{B}\Psi \in X \\ \forall \Psi \in X^{\perp}: \ H_0 \Psi \in X^{\perp}, \ \mathcal{B}\Psi \in X^{\perp} \end{cases} \tag{11}$$

The system can then be viewed as decomposed into two **independent** subsystems with wavefunctions $P\Psi$, $(I-P)\Psi$ (the projections of the total wavefunction Ψ to X and $X^{\perp}$). This decomposition can be further refined for any additional projection operator that commutes with H_0 and $\mathcal{B}$ to obtain a finite number of independent subsystems, each being associated with its L^2-projector P_1,...,P_K such that:

$$\begin{gathered} [H_0, P_i] = [\mathcal{B}, P_i] = 0, \ \forall i = 1, ..., K \\ \begin{cases} P_i P_j = 0, \ \forall i \neq j, \ i, j = 1, ...K \\ \sum_{i=1}^{K} P_i = I \end{cases} \end{gathered} \tag{12}$$

By using (10) for the projectors P_1,...,P_k one can prove that the system evolves on the product of hyper-spheres S_{Ψ_0}

$$S_{\Psi_0} = \{ f \in L^2(\mathbb{R}^{\gamma}); \|P_i f\|_{L^2(\mathbb{R}^{\gamma})} = \|P_i \Psi_0\|_{L^2(\mathbb{R}^{\gamma})}, \ i = 1, ..., K \} \tag{13}$$

Thus, we obtain conditions for controllability : if Ψ is reachable from Ψ_0 then Ψ is necessary in S_{Ψ_0}.

This example shows how the existence of conservation laws for the system introduce restrictions for controllability. For projectors to closed subspaces, the situation lends itself to an easy intuitive understanding. More complicated situations are possible when the conservation law in effect does **not** correspond to a projection and not even to a Hermitian operator. We may see this point through a simple example. Consider the 3-level system:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}, \ B = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{14}$$

and the corresponding evolution equations

$$\begin{aligned} i\frac{d}{dt}C_1(t) &= C_1(t) + \epsilon(t) C_2(t) \\ i\frac{d}{dt}C_2(t) &= 2C_2(t) + \epsilon(t) C_1(t) + \epsilon(t) C_3(t) \\ i\frac{d}{dt}C_3(t) &= 3C_3(t) + \epsilon(t) C_2(t) \end{aligned}$$

This system has degenerate transitions e.g. $\lambda_2 - \lambda_1 = \lambda_3 - \lambda_2$ and no $\mu \in \mathbb{R}$ can be found such that $A + \mu B$ comply with $\mathbb{HB}$ moreover no (non-trivial)

observable O exists that commutes with both A and B. Upon closer examination, a "hidden symmetry" is however found for this system. More precisely it is easy to prove that for any $t > 0$ and $\epsilon(t) \in L^2([0,t])$:

$$|C_1(t)C_3(t) - \frac{C_2(t)^2}{2}| = |C_{01}C_{03} - \frac{C_{02}^2}{2}|. \tag{15}$$

Therefore, if any controllability result is to be true for this setting, it must take into account the conservation law (15) ; any $\Psi(t) = \sum_{i=1}^{3} C_i(t)\Psi_i(x)$ that is reachable from $\Psi(0) = \sum_{i=1}^{3} C_{0i}\Psi_i(x)$ must satisfy the constraint (15). As an illustration of this point consider a simple numerical example. Suppose that the initial state is the ground state (Ψ_1) and the target is the first excited state (Ψ_2). A simple computation gives for Ψ_1 : $|C_{01}C_{03} - \frac{C_{02}^2}{2}| = |1 \cdot 0 - \frac{0^2}{2}| = 0$ and for Ψ_2 : $|C_1(t)C_3(t) - \frac{C_2(t)^2}{2}| = |0 \cdot 0 - \frac{1^2}{2}| = \frac{1}{2}$. Since the two quantities are different, one infers that Ψ_2 **is not reachable from** Ψ_1 and therefore the system is not controllable, despite the fact that the connectivity assumption $\mathbb{HA}$ is satisfied.

A detailed analysis of the case $N = 3$ shows that in each circumstance where the theorem 1 cannot be used, conservation laws are in effect. This leads us to state the following

Conjecture *As long as no new conservation laws appear –besides L^2 norm conservation – the system is controllable, i.e. any state on the unit sphere may be reached (in finite time and with finite energy) from any other.*

The statement above, if true, would have the merit of giving a controllability result independent of the mathematical transcription of the precise control situation (no mathematical properties of the matrices A and B are involved but only properties of the system they describe). When the Lie group corresponding to the Lie algebra generated by the internal Hamiltonian and the coupling matrix is a compact Lie group, a proof that appears to support the conjecture was communicated to us by V. Ramakrishna [29]. In general, it is not known whether the presence of conservation laws *prevents* controllability or only *restricts* the reachable set accordingly.

Remark 6 *Finite dimensional controllability results are only a part of the effort necessary for the theoretical understanding of quantum control problems. One still has to make compatible the* **positive** *results above or elsewhere ([14]) with the generic* **negative** *results for the infinite dimensional systems [20, 15, 21, 23]. The introduction of proper controllability concepts seems necessary to make further advances. Furthermore, it is interesting to note that usually when a quantum system is to be controlled the aim is not*

to precisely obtain a prescribed wavefunction, but rather to ensure that that some useful projections or expectation values have the desired behaviour.

Remark 7 *In the absence of positive infinite dimensional results, controllability conclusions based on some finite discretization should be treated with care. The number of eigenstates considered relevant to the control problem is important, as can be seen from the example in Eq. (14) : when discretized with only two eigenstates, the system is trivially controllable but the introduction of a third eigenstate generates the "hidden symmetry" with its associated loss of controllability. When the system is intrinsically infinite dimensional, the controllability of a low dimensional discretization does not imply the controllability of a larger (and more truthful) discretization involving all states that have important coupling matrix elements with the low dimensional space or domain of interest. As with numerical wave packet modelling calculations, it is suggestive that convergence of controllability conclusions may also occur within the domain of interest as the overall space is expanded in dimension.*

5 Conclusions

Wavefunction controllability of finite dimensional quantum systems interacting with external fields was explored from a practical perspective suggested by recent theoretical results [16]. The criteria presented was seen to be useful for a wide range of problems and very easy to check. Systems with unusual conservation laws that prevent controllability were also presented and the relationship with the theoretical criteria was investigated. Open questions with positive answers in some particular cases were stated as a conjecture. Numerical experiments were undertaken to illustrate the theoretical results and the connection with optimal control theory was discussed. The assessment of controllability is fundamental to the manipulation of quantum systems. Some tools are now available to make this assessment, but a full comprehensive analysis still needs to be developped.

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