Proceedings of the 39th IEEE
Conference on Decision and Control
Sydney, Australia • December, 2000

Constructive controllability for systems with drift motivated by and applied to quantum control

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Abstract

The purpose of this paper is fourfold: i) First, a brief description of how finite dimensional models arise in quantum control will be given. ii) Second, many notions in quantum engineering such as universality of logic gates, hard pulse approximation in NMR spectroscopy etc., will be related to controllability of systems on the unitary groups. iii) Recent results, of the authors, on constructive controllability, in the class of piecewise constant controls with constraints placed on them, for systems with drift on the unitary groups will be sketched. iv) Finally, a **new** decomposition of $SU(2)$ matrices will be provided and used to illustrate how problems caused by periodicity arguments, to address the presence of drift, may be circumvented.

1 Introduction

Several applications call for the control of quantum systems. Examples are: i) Molecular control or site-specific photochemistry, in which molecules are irradiated with electromagnetic fields so as to enhance product specificity or to enable spectroscopy, [1, 6]; i-i) Lasing Without Inversion (LWI) in which the lasing action is achieved without putting bulk of the population in the *unstable* higher energy state as opposed to the conventional practice, [2]; iii) NMR spectroscopy, [7, 13]; iv) Quantum information systems - the construction of quantum logic gates and cryptosystems, [17]. In one form or the other all these problems can be reduced to the problem of state preparation for a quantum system to a desired final state. The second problem, **LWI**, illustrates this. The resolution of this problem proceeds as follows. Call the ground state, x_1 and the excited state, x_2. Choose another state x_3, higher in energy than the ground state. Then drive the quantum system via an external field to go from the state $(1,0,0)$ to a state (c_1, c_2, c_3). The superposition of coherent states (c_1, c_2, c_3) is so chosen that amplification is maximized while keeping, $\mid c_2 \mid$, the population in the excited state at a minimum. *The idea is that this superposition will create two interfering pathways (thus, mimicking the double slit experiment) and manipulation of these intereferences will lead to amplification.* Manipulation of such coherent superpositions(in some cases these superpositions live in tensor product spaces - known as entangled states) is the essential feature of all quantum control problems.

Before proceeding, a note about the bibliography is appropriate. For reasons of length only immediately relevant papers are cited, and in most cases survey articles which have extensive bibliographies have been preferred.

2 Finite Dimensional Models:

One may be lead to believe that quantum control is the control of a partial differential equation (the Schrodinger equation) and thus belongs to the purview of distributed parameter systems. While there are examples which call for an infinite dimensional analysis (see e.g., [3]), this viewpoint is narrow. In fact, if one goes through the derivation of most of the partial differential equations of physics, it becomes clear that the passage to a partial differential equation is itself an approximation. Thus, there is no reason *a priori* to believe that a PDE model is more accurate than a finite dimensional model. Many quantum phenomena have been very accurately described by finite dimensional models. Predictions based on such models have been experimentally confirmed.

Thus, the viewpoint being espoused in this paper is

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that the system being controlled is assumed to be described by unitary evolution in a complex Hilbert space whose dimension is the maximum number of independent states that can be distinguished by the experiment. For instance, spin systems evolve in finite dimensional spaces, because magnetic fields cannot excite other modes. Similarly, microwave fields usually only cause rotations and we can thus ignore vibrations, electronic transitions etc., Of course, many of these finite dimensional models are valid under certain assumptions. These assumptions have to be met by the control field to prevent the analogue of the spillover effect. *Thus most controllability questions that have to be studied are constrained controllability problems.*

In what follows we provide a few "mathematical" justifications of the usage of finite dimensional systems. Suppose that the original problem was given via:

$$i\hbar\dot{\psi} = (H_0 + V(x))\psi + H_{ext}\psi$$

In the above equation, x is the spatial coordinate and $\hbar$ is $\frac{h}{2\pi}$ (h is Planck's constant). By passing to atomic units, one may take $\hbar = 1$. Further, $H_{int} = H_0 + V(x)$ is the internal Hamiltonian, with H_0 being the kinetic energy and $V(x)$ the potential energy. H_{ext} is the external Hamiltonian (this contains the control term). For molecular control problems, for instance, H_{ext} is given by $-\mu(x)\epsilon(t)$. $\mu(x)$ is the dipole operator and $\epsilon(t)$ is the external real valued electromagnetic field.

Passage to a finite dimensional model is formally justified by expanding the wave function $\psi(x,t)$ as a finite sum of the form $\sum_{k=1}^{n} c_k(t)\phi_k(x)$. The $\phi_k(x)$ are usually taken to be the eigenfunctions of the operator $H_0 + V(x)$. Plugging this into Schrodinger's equation results in a bilinear control system

$$\dot{c} = Ac + Bcu(t); c(0) = c_0 \qquad (1)$$

The state of this system is $c = (c_1, \ldots, c_n)$ and has the interpretation of being probability amplitudes. Hence c takes values in a sphere.

The following is a short list of situations which justify the use of finite dimensional models: i) Many of the symmetry groups of quantum mechanical Hamiltonians are compact. Thus, a certain problem often lives in some irreducible representation of the group, which is finite dimensional. Many examples of this may be found in [5]. For instance, the chemical properties of nitrogen can be described by a system evolving unitarily in a 20 dimensional space. Similarly, the electronic properties of buckminsterfullerene are essentially described by a system evolving in a 60 dimensional space. ii) For many problems the operator, $(H_0 + V(x)) - \mu(x)$ can be shown to leave a finite dimensional subspace of the space of square integrable functions invariant. This leads to finite dimensional models. This forms the basis of the so called algebraic approach to molecular dynamics, [10]. A related situation is that H_{int}, H_{ext} belong to a finite dimensional Lie algebra of operators. Passage to the Heisenberg picture then leads to a finite dimensional system; iii) Assumptions about the spectrum of the control allows us to neglect many modes. For instance, *ultra-violet* radiations do not cause vibrational transitions. This combined with other approximations such as the Born-Oppenheimer approximation, [12], leads to finite dimensional models. iv) There are reasons to believe that space is essentially "grainy" and thus quantum mechanics should be studied on a lattice instead of a continuum, [23]. The appropriate Hilbert space then is set of L^2 functions on a lattice. These latter spaces are of course just some C^N, and thus the corresponding quantum mechanics is finite-dimensional.

Thus, we are lead to consider constrained state preparation problems for the bilinear system (1). As usual it is is better to consider the evolution of the transition matrix:

$$\dot{U} = AU + BUu(t), U(0) = I_N, U \in U(N) \qquad (2)$$

Due to the results of [4] we know theoretically that not only controllability, but also constrained and bang-bang controllability, can be ensured under appropriate conditions. However, the system under study has drift and there are not many explicit techniques for producing controls which effect the desired state transfer. The few techniques which admit a drift work under circumstances which are not applicable to our problem. For a survey of what is known about constructive controllability for classical systems we refer the reader to [11]. The potentially general technique of exploiting periodicity to overcome drift is flawed. Thus, the results of this paper are relevant not only for quantum systems but also for classical mechanical systems. [19] provides an example of an application of quantum techniques to a classical systems.

3 Controllability, Universality and Hard Pulses

The purpose of this section is to show how notions such as universality of logic gates in quantum computation, and the hard pulse approximation in nuclear magnetic resonance spectroscopy are consequences of the results of, [4] on the controllability of invariant systems on compact Lie groups.

Universality of Logic Gates: In [21] it is argued heuristically that a generic pair of $N \times N$ anti- Hermitian matrices is universal for quantum computing since generically the Lie algebra generated by A, B is $u(N)$. Thus, every matrix $U \in U(N)$ can be obtained by "switching on and off" two Hamiltonians (those represented by A and B) - whence the terminology, " univer-

sal". In [22] the authors conjecture that if $A, B \in u(N)$ have the above Lie algebra generating property then every $U \in U(N)$ can be generated by switching on and off a single Hamiltonian (A representing the switched off Hamiltonian and B the switched on Hamiltonian).

In [14] the relation between universality and the results of [4] was pointed out. Since [14] was required to be short (a page and a half) we will provide a quick proof of this connection here. See [20] for a different proof.

Since [21] does not explicitly write down the equation representing the dynamics of the system, the quickest way of obtaining its results are to interpret it as the results of [4] on unconstrained controllability for the driftless system:

$$\dot{U} = AUu_1(t) + BUu_2(t)$$

To obtain the results of [22, 20] we have to consider a system with drift

$$\dot{U} = AU + CUu(t), A, C \in u(N)$$

Then, the phraseology of [22, 20] makes it clear that A represents the above system with the input $u(t) = 0$ and $B = A + C$, represents the system with the input $u(t) = 1$. Hence, we would be done if we can show that the Lie algebra generating condition implies bang-bang controllability (with controls being either 0 or 1). In [4] this is shown to be true of the control values are 1 and -1. However, this implies the desired bang-bang controllability. Indeed, introduce new control, $v(t) = 2u(t) - 1$. Then if $u(t)$ takes values 0 or 1 then $v(t)$ takes values -1 or 1. In terms of v the control system reads as:

$$\dot{U} = (A - C)U + 2CUv(t)$$

Clearly if the Lie algebra generated by A and B is all of $u(N)$ then so is the Lie algebra generated by $A - C = A - (B - A) = 2A + B$ and $2C = 2(B - A)$. This completes the argument.

Hard Pulse Approximation: In NMR spectroscopy the following argument is frequently given. Assume that A and B are two skew Hermitian matrices which represent the free evolution and the control coupling respectively of the system. Thus, the system under consideration is of the form

$$\dot{c} = Ac + Bcu(t)$$

The above model is usually valid in the absence of the relaxation effect (see [13]). If one probes the system with a constant pulse of high amplitude, then one may neglect the A term in the evolution, so that the evolution of the corresponding transition matrix is essentially given by e^{Bkt} where k is a constant much larger than one in absolute value. This is the so called hard pulse approximation. The claim then is that every $N \times N$ unitary matrix U can be generated by a combination of free evolution and hard pulses,

This can be formally shown to be valid. Indeed, consider an auxilliary system;

$$\dot{U} = AU + (B - A)Uu(t)$$

Now if the Lie algebra spanned by A and B is $u(N)$ then the same is true of the Lie algebra spanned by A and $B - A$. Thus, this auxilliary system is controllable. By [4] it follows that every U can be generated by controls which only take the values 0 and 1. The time evolution corresponding to a 0 pulse is given by an exponential of A, whereas that corresponding to the control 1 is an exponential of B. So we get the result that every U can be written as a product of exponentials of A and B with positive coefficients. Note that no high amplitude controls are needed for this argument. Indeed, high amplitude controls render extending the hard pulse argument difficult for homonuclear systems.

4 Constructive Controllability on the Unitary Groups

Motivated by the discussion of the preceeding subsections, we now address the following abstract problem:

Problem: Given an element $S \in SU(2)$ and two linearly independent elements $A, B \in su(2)$, find a decomposition $S = \Pi_{k=1}^{Q} e^{(a_k A + b_k B)}$ so that:

- **O1**: $a_k \geq 0$ for all k, and $a_k > 0$ if $b_k \neq 0$ (*Constructive Controllability*).
- **O2**: $\mid b_k \mid \leq C$ for some *a priori* prescribed bound C, in addition to **O1** (*Constructive Bounded Controllability*).
- **O3**: $b_k = 0$ or $b_k = a_k$ for all k, in addition to **O1** (*Constructive Bang-Bang Controllability*)

The number of factors, Q, **is not** required to be the same for every objective above.

The terminology used in this problem can be justified by considering the preparation of the target S, via piecewise constant controls, for the system:

$$\dot{U} = Au + BUu(t), U(0) = I_2 \qquad (3)$$

Before a concrete result is presented on the above problem, a few comments are in order.

a)The reason for studying systems on $SU(2)$ are i) this already covers several important applications including even classical systems, and ii) systems on higher dimensional unitary groups may often be addressed via

$SU(2)$ methods in combination with approximations, [15]. Furthermore, there are several features of the 2 dimensional case which carry over to the higher dimensional case (i.e., when one does not resort to approximations). In the higher dimensional case calculations are naturally more arduous, and hence $SU(2)$ is a good starting point. **b)** $SU(2)$, and not $U(2)$ was chosen since either i) many examples are already in this form as in the case of the control of electron spin; or ii) it amounts to only neglecting an overall phase which is physically irrelevant, [16]. **c)** The desired factorizations are also relevant for non piecewise constant controls. Typically, other classes of controls are handled via approximations such as averaging or the rotating wave approximation, [12]. An example of an N-level system controlled via sinusoidal controls is provided in [15], Notice that, depending on the approximation, the interpretation of a_k and b_k will be different. For instance they may represent the duration and average of a pulse or the phase and pulse area of a periodic pulse.

Theorem 4.1 *Let A and B be two linearly independent elements of $su(2)$. Then i)* **O1** *can be achieved with Q at most 4 for any $S \in SU(2)$. If in addition, A and B are orthogonal then* **O2** *can be achieved with Q depending only on the target S and the bound C. Finally, if A and B are orthonormal then* **O3** *can be achieved with Q at most 35 for any S.*

Sketch of the Proof: The proof is sketched. For further details see [16, 18]. The basic idea is to map the given pair A and B, via a Lie algebra isomorphism ψ^{-1} onto the drift and control vector fields of an orthonormal pair $\hat{A}, \hat{B}$, respectively, for which the desired objective has been met. To ensure that the map ψ (there is just one choice for this map ψ) is a Lie algebra isomporphism we require A and B to be orthonormal. Orthogonality can be achieved by a preliminary control and the additional normalization can be obtained by scalings. Clearly, a preliminary control or a scaling does not affect **01**. However, a preliminary control precludes **O2**, while a scaling does not. Both scaling and preliminary controls do not respect **O3**.

Armed with ψ, the achievement of these 3 objectives follows the steps below: **S1**: Find the logarithm of S and express it as a linear combination $c_1A + c_2B + c_3[A,B]$ for some real constants $c_i, i = 1,\ldots,3$. **S2**: Associate to S the matrix $T = exp(c_1\hat{A}+c_2\hat{B}+c_3[\hat{A},\hat{B}])$ Thus, it holds that $\phi(T) = S$, where $\phi : SU(2) \to SU(2)$ is the Lie group homomorphism associated to the Lie algebra isomorphism ψ. **S3**: Achieve **O1, O2** and **O3** for the system

$$\dot{U} = \hat{A}U + \hat{B}Uu(t)$$

and the target T. Then, by virtue of the way ψ and ϕ are defined it follows that the same a_k, b_k, Q which worked for the pair A, B and the target T work for the pair A, B and the target S.

For **O1, O2** choose $\hat{A} = \frac{i}{2}\sigma_z, \hat{B} = \frac{i}{2}\sigma_y$, while for **O3** the pair $\frac{i}{2}\sigma_z, \frac{i}{2}\sigma_x$ was chosen. Details of the specific formulae of a_k, b_k in terms of the elements of T (and, thereby S) may be found in [16, 18]. While the Q for **O2** and **O3** could conceivably be improved by making better choices for $\hat{A}$ and $\hat{B}$, it is our belief that the bound on Q for **O1** cannot be improved. Indeed, for reasons of dimension ($SU(2)$ is three dimensional) at least 3 factors can be expected for a general $S \in SU(2)$ if the a_k, b_k are not restricted to meet **O1**. Further imposition of the **O1** requirement is bound to increase the number of factors. So 4 is indeed an optimal bound for Q for the objective **O1**.

For several specific examples the orthonormality condition can be relaxed. One special case is when $A = ia\sigma_x + ib\sigma_y, B = ic\sigma_x + id\sigma_y$, [16]. It is not assumed that A and B are orthonormal. Such examples arise in the control of the electron spin and in classical systems such as switched networks. In [18, 19] it is shown how to meet even **O3** (Constructive Bang-Bang Controllability) for certain switched network examples without any preliminary control or scalings. Furthermore, the number of factors required to achieve **O3**, in these network examples, is three, [19]. Thus, where the general approach would not even have been applicable an intrinsic approach to such pairs achieves **O3** with far fewer than 35 factors.

Finally, by modifying the central idea of the proof one can obtain similar results on systems evolving on the orthogonal groups $SO(3)$ and $SO(4)$, [16, 18, 19]. These latter groups are related to $SU(2)$ and it is this relation that is exploited in these references. Many classical systems have all or part of their evolution defined on $SO(3)$. The groups $SO(n)$ arise also in the description of switched electrical circuits, [9] (where n is the number of circuit elements).

5 A New Decomposition of $SU(2)$ to Overcome Periodicity:

One natural method, that is tempting to adopt in the presence of drift, is to use periodicity along with constructive techniques for the following driftless system:

$$\dot{U} = AUu_1(t) + BUu_2(t) \tag{4}$$

Constructively controlling this driftless system amounts to factoring every $S \in SU(2)$ as $\Pi_{i=1}^{V} e^{(a_kA+b_kB)}$ without requiring that a_k be positive. It would seem that this can be used to achieve at least **O1** for (3) in the following way. Consider the typical factor, $e^{(a_kA+b_kB)}$. The matrix being exponentiated - call it C_k for brevity

- satisfies $e^{C_k t} = e^{C_k(t+nP)}$ for some period P and all integers n. Thus $e^{C_k} = e^{C_k(1+nP)}$. If $a_k \leq 0$, it is plausible that by making an appropriate choice for n that the new coefficient of the drift, namely $a_k(1+nP)$ is positive, thus providing objective **O1** for (3). This strategy has at least three drawbacks: **D1:** It does not work for factors whose corresponding drift coefficient, a_k, is 0. No amount of periodicity will render a zero drift coefficient into a non-zero drift coefficient. **D2:** Even for terms where this strategy works, it may be deleterious because it may require the application of a pulse for a long time and thereby causing the pulse area, $\mid b_k \mid$, to be large. While for mechanical systems this may only be a practical hindrance, for quantum systems it is also a serious theoretical drawback because this may cause many approximations, such as neglecting other levels and physical processes, to break down. **D3:** This method fails even more in higher dimensions because the typical element of $su(N), N \geq 3$ does not have a periodic flow. In the results presented above periodicity is only used to rewrite free evolution terms with negative drift coefficients as free evolution terms with positive drift coefficients, and even these instances are kept to a minimum. A **new** factorization of $SU(2)$ is presented along with an example which illustrates how to overcome **D2**.

For the purposes of explaining the proposed decomposition, the following notation is useful. Given a complex number γ, denote by $\bar{\gamma}$ its complex conjugate, and then define: $V(\gamma) = \exp \begin{pmatrix} 0 & i\gamma \\ i\bar{\gamma} & 0 \end{pmatrix}$ In [15] the following facts were established:

Proposition 5.1 *i) Writing any $S \in SU(2)$ in the representation,*

$$S = S(\alpha, \zeta, \mu) = \begin{pmatrix} e^{i\zeta}\cos\alpha & e^{i\mu}\sin\alpha \\ e^{i(\pi-\mu)}\sin\alpha & e^{-i\zeta}\cos\alpha \end{pmatrix}$$

we have $S = V(\alpha e^{i(\zeta+\mu-\frac{\pi}{2})})e^{i\lambda\sigma_z}$.; and ii) For any $L \in R$, in particular ζ it holds that $e^{iL\sigma_z} = V(\gamma_1)V(\gamma_2)$, with the complex numbers given by $\gamma_k = \frac{\pi}{2}e^{i\theta_k}, k = 1, 2$. with $L = \theta_1 - \theta_2 + \pi$.

Note that this proposition is **not** the Euler decomposition as the complex numbers $\gamma_k, k = 1, 2, 3$ need not be purely real nor purely imaginary.

Consider the following example. Let $A = i\sigma_y$ and $B = i\sigma_x$. Suppose the desired target is $e^{(-i\sigma_y + i\sigma_x)}$. This target can be achieved for the associated driftless system by choosing $u_1(t) = -1, u_2(t = 1$ applied for $T = 1$ unit of time (note this is exactly what one would get if the Proposition (5.1) was formally applied). Exploiting periodicity in this context means that the flow of the vector field $C = -A + B$ is periodic of period $\sqrt{2}\pi$ and thus $e^C = e^{C(1-\sqrt{2}\pi)}$. Now $e^{C(1-\sqrt{2}\pi)} = e^{-[(1-\sqrt{2}\pi)A + (1-\sqrt{2}\pi)B]}$. Thus, **O1** has been achieved for the given system (which has drift) bu using a single pulse with pulse area (i.e., the corresponding $\mid b_k \mid$) $\sqrt{2}\pi - 1$.

We will now use a **different** method. First notice that:

$$S(\alpha, \zeta, \mu) = S(\frac{\pi}{2} - \alpha, \mu + \pi, \zeta) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad (5)$$

The utility of (5) is that if the γ_1 of Proposition (5.1), corresponding to $S(\alpha, \zeta, \mu)$, lies in any half-plane then the γ_1 corresponding to $S(\frac{\pi}{2} - \alpha, \mu + \pi, \zeta)$ lies in the complementary half-plane. This is precisely what is needed to ensure that the coefficients of the drift term are positive. Thus, if the γ_1 corresponding to $S(\alpha, \zeta, \mu)$ does not have drift coefficient, a_1, positive then the a_1 corresponding to $S(\frac{\pi}{2} - \alpha, \mu + \pi, \zeta)$ will be positive, since the two corresponding θ_1's differ by π. Note that the remaining two γ's never pose a problem since the relation $L = \theta_2 - \theta_3 + \pi$ and the fact that L can always be taken to be in $[0, 2\pi)$ means that γ_2 and γ_3 can always be chosen to belong to the same open half plane.

Returning to the example notice that the target is $S(\sqrt{2}, 0, \frac{5\pi}{4})$. Hence Proposition (5.1) cannot be directly used since the corresponding γ_1 is in the wrong quadrant. However, using Equation (5 leads to $S = S(\frac{\pi}{2} - \sqrt{2}, \frac{\pi}{4}, 0) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. The second factor can be obtained by free evolution, and hence with zero pulse area. Applying Lemma to the first factor we get that it is equal to $V(\gamma_1)V(\gamma_2)V(\gamma_3)$ where $\gamma_1 = (\frac{\pi}{2} - \sqrt{2})e^{i\frac{5\pi}{4}}$. This corresponds to a pulse, of pulse area $\frac{\frac{\pi}{2}-\sqrt{2}}{\sqrt{2}}$, applied for $\frac{\frac{\pi}{2}-\sqrt{2}}{\sqrt{2}}$ units of time. Choosing $\gamma_2 = \frac{\pi}{2}e^{i\frac{\pi}{2}}$ and $\gamma_3 = \frac{\pi}{2}e^{i\frac{5\pi}{4}}$, leads to zero pulse area for the second factor and pulse area equal to $\frac{\pi}{2\sqrt{2}}$ for the third factor.

Notice that, by virtue of this new decomposition, even the cumulative pulse area is lower than that required by the use of periodicity.

This decomposition of $SU(2)$, based on Equation (5), was not used in [16] since a different decomposition turned out to be even more versatile. However, the decomposition in this paper is better suited for minimizing the cumulative pulse area while respecting **O1**.

6 Acknowledgements

Th research of the first and the last author was supported in part by NSF - DMS 0072415 and NSF -DMS 9803186 respectively. The third author was supported in part by NSF and DOD. The first author is grateful to his parents for their encouragement and support.

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