Algorithms for Quantum Control without Discontinuities; Application to the Simultaneous Control of two Qubits

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Abstract

We propose a technique to design control algorithms for a class of finite dimensional quantum systems so that the control law does not present discontinuities. The class of models considered admits a group of symmetries which allows us to reduce the problem of control to a quotient space where the control system is 'fully actuated'. As a result we can prescribe a desired trajectory which is, to some extent, arbitrary and derive the corresponding control. We illustrate this technique with examples and focus on the application to the simultaneous control of two non-interacting spin $\frac{1}{2}$ particles with different gyromagnetic ratios in zero field nuclear magnetic resonance (NMR). Our method provides a flexible toolbox for the design of control algorithms to drive the state of finite dimensional quantum systems to any desired final configuration, with smooth controls.

Keywords: Control Methods for Quantum Mechanical Systems; Smooth Control Functions; Symmetry Reduction; Nuclear Magnetic Resonance.

1 Introduction

The combination of control theory techniques with quantum mechanics (see, e.g., [13], [17], [19]) has generated a rich set of control algorithms for quantum mechanical systems modeled by the Schrödinger (operator) equation

$$\dot{X} = AX + \sum_{j=1}^{m} B_j u_j X, \qquad X(0) = \mathbf{1}. \tag{1}$$

Here we assume that we have a finite dimensional model, A and B_j are matrices in $\mathfrak{su}(n)$ for each $j = 1, ..., m$, X is the unitary propagator, which is equal to the identity $\mathbf{1}$ at time zero, and u_j are the controls. These are usually electromagnetic fields, constant in space but possibly time-varying, which are the output of appropriately engineered pulse-shaping devices. Many of the proposed algorithms in the literature involve control functions which are only piecewise continuous and in fact have 'jumps' at certain points of the interval of control. For example, control algorithms based on *Lie group decompositions* (see, e.g., [23]) involve 'switches' between different Hamiltonians ($A + \sum_j B_j$ in (1)); Algorithms based on *optimal control*, even if they produce smooth control functions, often require a jump at the beginning of the control interval in order for the control to achieve the prescribed value in norm (assuming a bound in norm of the optimal control as in [15]). Beside the practical problem of generating (almost) instantaneous switches with pulse shapers, such discontinuities introduce undesired high frequency components in the dynamics of the controlled system. For these reasons, it is important to have algorithms which produce *smooth* control functions whose values at the beginning and the end of the control interval are equal to zero.

This paper describes a method to design control functions without discontinuities in order to drive the state of a class of quantum systems of the form (1) to an arbitrary final configuration. Our main example of application will be the simultaneous control of two quantum bits, a system which was also considered in [20] (in zero field nuclear magnetic resonance (NMR)) and [14], in the context of optimal control. As compared to these papers, we abandon here the requirement of time optimality (under the constraint of bounded norm for the control) but introduce a novel method which will allow us more flexibility in the control design. The result is a control algorithm that does not present discontinuities, with the control equal to zero at the beginning and at the end of the control interval.

The paper is organized in two main sections each of which divided into several subsections. In Section 2 we describe the class of systems we consider and the general theory underlying our method. We also present two simple examples of quantum systems where the theory applies. In Section 3 we detail the application to the system of two spin $\frac{1}{2}$ particles in zero field NMR above mentioned.

2 General Theory

2.1 Class of systems considered

Consider the class of control systems (1) with A and B_j, $j=1,...,m$, in $\mathfrak{su}(n)$ and let $\mathcal{L}$ denote the Lie algebra generated by $\{A, B_1, ..., B_m\}$. We assume that $\mathcal{L}$ is semi-simple, which implies, since $\mathcal{L} \subseteq \mathfrak{su}(n)$, that the associated Lie group $e^{\mathcal{L}}$ is compact. The Lie algebra $\mathcal{L}$ is called, in quantum control theory, the *dynamical Lie algebra* associated to the system (1). Since $e^{\mathcal{L}}$ is compact, the Lie group $e^{\mathcal{L}}$ is the set of states for (1) reachable by changing the control [21]. In particular if $\mathcal{L} = \mathfrak{su}(n)$, the system is said to be *controllable* because every special unitary matrix can be obtained with appropriate control. These are known facts in quantum control theory (see, e.g., [17]). We assume that $\mathcal{L}$ has a (vector space) decomposition $\mathcal{L} = \mathcal{K} \oplus \mathcal{P}$, such that $[\mathcal{K}, \mathcal{K}] \subseteq \mathcal{K}$, i.e., $\mathcal{K}$ is a *Lie subalgebra of* $\mathcal{L}$, which we also assume to be semisimple so that $e^{\mathcal{K}}$ is compact. Moreover $[\mathcal{K}, \mathcal{P}] \subseteq \mathcal{P}$. A special case is when, in addition, $[\mathcal{P}, \mathcal{P}] \subseteq \mathcal{K}$ in which case the decomposition $\mathcal{L} = \mathcal{K} \oplus \mathcal{P}$ defines a symmetric space of $e^{\mathcal{L}}$ [22]. We assume, in the model (1), that such a decomposition exists so that $A \in \mathcal{K}$ and $\{B_1, ..., B_m\}$ forms a basis for $\mathcal{P}$.

Under such circumstances, we can reduce ourselves to the case $A = 0$ in (1), i.e., to systems of the form

$$\dot{U} = \sum_{k=1}^{m} \hat{u}_k B_k U, \qquad U(0) = \mathbf{1}. \tag{2}$$

To see this, assume that for any fixed interval $[0, t_f]$ and any desired final condition U_f, we are able to find a control $\hat{u}_k$, defined in $[0, t_f]$, steering the state U in (2) from the identity $\mathbf{1}$ to U_f. Let $a_{kj} = a_{kj}(t)$, $k, j = 1, ..., m$ the coefficients forming an $m \times m$ orthogonal matrix, so that, for any $j = 1, ..., m$,

$$e^{-At} B_j e^{At} = \sum_{k=1}^{m} a_{kj}(t) B_k. \tag{3}$$

Let X_f be the desired final condition for (1) and $\hat{u}_k$ be the control steering the state U of system (2) from the identity $\mathbf{1}$ to $e^{-At_f} X_f$, in time t_f. Then the control u_j obtained inverting

$$\hat{u}_k(t) := \sum_{j=1}^{m} a_{kj}(t) u_j(t), \tag{4}$$

steers the state X of (1) from the identity to X_f. This follows from the fact that, if $U = U(t)$ is the solution of (2) with the control $\hat{u}_k$, and final condition $e^{-At_f} X_f$, then $X = e^{At} U$ is a solution of (1), with the controls u_j given by (4) and therefore the final condition at t_f is X_f. Notice that the transformation (4) does not modify the smoothness properties of the control, neither does it modify the fact that the control is zero at the beginning and at the end of the control interval (or at any other point). Therefore in the following we shall deal with *driftless systems* of the form (2) with the Lie algebraic $\mathcal{L} = \mathcal{K} \oplus \mathcal{P}$, structure above described. In particular $\{B_1, ..., B_m\}$ forms a basis for $\mathcal{P}$.

2.2 Symmetry reduction

The compact Lie group $e^{\mathcal{K}}$ can be seen as a Lie transformation group which acts on $e^{\mathcal{L}}$ via conjugation $X \in e^{\mathcal{L}} \to KXK^{-1}$, $K \in e^{\mathcal{K}}$. Moreover this is a *group of symmetries* for system (2) in the sense that, for every $K \in e^{\mathcal{K}}$, $KB_jK^{-1} \in \mathcal{P}$ for each j. In particular let $KB_jK^{-1} := \sum_{k=1}^m a_{kj}B_k$ for an orthogonal matrix $\{a_{kj}\}$ depending on $K \in e^{\mathcal{K}}$ (cf. (3)). If $U = U(t)$ is a trajectory corresponding to a control $\hat{u}_k$, KUK^{-1} is the trajectory corresponding to controls $u_k := \sum_{j=1}^m a_{kj}\hat{u}_j$, as it is easily seen from (2) and

$$K\dot{U}K^{-1} = \sum_{j=1}^m \hat{u}_j KB_jK^{-1}KUK^{-1} = \sum_{j=1}^m \hat{u}_j \left(\sum_{k=1}^m a_{kj}B_k\right) KUK^{-1} =$$

$$= \sum_{k=1}^m \left(\sum_{j=1}^m a_{kj}\hat{u}_j\right) B_kKUK^{-1} = \sum_{k=1}^m u_kB_kKUK^{-1}.$$

Therefore, if we find a control steering the state U of (2) to some $\hat{U}_f$ a *'rotated' control* obtained by similarity transformation with a $K \in e^{\mathcal{K}}$, we will obtain state transfer to U_f in the same orbit as $\hat{U}_f$. This suggests to treat the control problem on the *quotient space* $e^{\mathcal{L}}/e^{\mathcal{K}}$ corresponding to the above action of $e^{\mathcal{K}}$ on $e^{\mathcal{L}}$.

From the theory of Lie transformation groups (see, e.g., [16]), we know that the quotient space $e^{\mathcal{L}}/e^{\mathcal{K}}$ has the structure of a *stratified space* where each stratum corresponds to an *orbit type*, i.e., a set of points in $e^{\mathcal{L}}$ which have conjugate isotropy groups. The stratum corresponding to the smallest possible isotropy group, K_{min}, is known to be a connected manifold which is *open and dense* in $e^{\mathcal{L}}/e^{\mathcal{K}}$. We denote it here by $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$, where *reg* stands for the *regular* part. Its preimage in $e^{\mathcal{L}}$, $e^{\mathcal{L}}_{reg}$, under the natural projection $\pi : e^{\mathcal{L}} \to e^{\mathcal{L}}/e^{\mathcal{K}}$ is open and dense in $e^{\mathcal{L}}$ as well. It is analogously called the *regular part* of $e^{\mathcal{L}}$. The complementary set in $e^{\mathcal{L}}/e^{\mathcal{K}}$, (resp. $e^{\mathcal{L}}$) is called the *singular part*. The dimension of $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$ as a manifold is

$$\dim(e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}) = \dim(e^{\mathcal{L}}) - \dim(e^{\mathcal{K}}) + \dim K_{min} = \dim(\mathcal{L}) - \dim(\mathcal{K}) + (\dim K_{min}), \tag{5}$$

where $\dim(K_{min})$ is the dimension of the minimal isotropy group as a Lie group [1]. In particular, if K_{min} is a *discrete Lie group*, i.e., it has dimension zero, the right hand side of (5) is the dimension of the subspace $\mathcal{P}$. This is verified for instance in $K - P$ problems when $e^{\mathcal{L}} = SU(n)$ (cf., e.g., [18]). We shall assume this to be the case in the following.

According to a result in [18], under the assumption that the minimal isotropy group K_{min} is discrete, the restriction of π_* to $R_{x*}\mathcal{P}$ is an isomorphism onto $T_{\pi(x)}\left(e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}\right)$ for each point x in the regular part, $e^{\mathcal{L}}_{reg}$. Here, as it is often done, we have identified the Lie algebra $\mathcal{L}$ with the tangent space of $e^{\mathcal{L}}$ at the identity $\mathbf{1}$, and therefore $\mathcal{P}$ is identified with a subspace of the tangent space at $\mathbf{1}$. The map R_x is the *right translation* by x so that $R_{x*}\mathcal{P}$ is a subspace (with the same dimension of $\mathcal{P}$) of the tangent space at x, $T_xe^{\mathcal{L}}$ [2]. In Appendix B, we show that in given coordinates the determinant of the restriction of π_* to $R_{x*}\mathcal{P}$ is invariant under the action of $e^{\mathcal{K}}$. The above isomorphism result says that in the regular part $\det \pi_* \neq 0$. In this situation, for every regular point $U \in e^{\mathcal{L}}$, for every tangent vector $V \in T_{\pi(U)}(e^{\mathcal{L}}_{reg}/e^{\mathcal{K}})$, we can find a tangent vector $\pi_*^{-1}V \in R_{U*}\mathcal{P}$. Such a tangent vector is *horizontal* for system (2) which means that it can be written as a linear combination of the available vector fields $\{B_k U\}$ in (2). If $\Gamma = \Gamma(t)$ is a curve entirely contained in $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$ and $U = U(t)$ a curve in $e^{\mathcal{L}}_{reg}$ such that $\pi(U(t)) = \Gamma(t)$ for every t, i.e., U is a '*lift*' of Γ, then $\pi_*|_U^{-1}\dot{\Gamma}$ is a horizontal tangent vector at $U(t)$ for every t. If Γ joins two points Γ_0 and Γ_1 in $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$, in the interval $[t_0, t_1]$, and U_0 is such that $\pi(U_0) = \Gamma_0$, then the solution of the differential system

$$\dot{U} = \pi_*|_U^{-1}\dot{\Gamma}, \qquad U(t_0) = U_0, \tag{6}$$

is such that $\pi(U(t_1)) = \Gamma_1$. Therefore, once we prescribe an arbitrary trajectory Γ to move in the quotient space between two given orbits Γ_0 and Γ_1 in the regular part, the control specified by

$$\pi_*|_U^{-1}\dot{\Gamma} = \sum_{j=1}^{m} u_j B_j U \tag{7}$$

will allow us to move between two states U_0 and U_1 such that $\pi(U_0) = \Gamma_0$ and $\pi(U_1) = \Gamma_1$.

2.3 Methodology for Control

The above considerations suggest a general methodology to design control laws for systems of the form (2). In fact, given the freedom in the choice of the trajectory $\Gamma = \Gamma(t)$ above mentioned, we can design such control laws satisfying various requirements and, in particular, without discontinuities. Such a methodology can be summarized as follows.

First of all we need to obtain a geometric description of the orbit space $e^{\mathcal{L}}/e^{\mathcal{K}}$, and in particular of its regular part $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$. This was obtained for a large class of systems in [12]. Furthermore, we verify that the minimal isotropy group, which is the isotropy group of the elements in $e^{\mathcal{L}}_{reg}$, is discrete so that the right hand side of (5) is equal to $\dim \mathcal{P}$. This is a weak assumption, easily verified in the examples that will follow and that can be proven true in several cases [18], [24]. Then one chooses coordinates for the manifold $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$. These are expressed in terms of the original coordinates in $e^{\mathcal{L}}$ or, more commonly, in terms of the entries of the matrices in $e^{\mathcal{L}}$. Such coordinates are a complete set of *independent invariants* with respect to the (conjugacy) action of the group $e^{\mathcal{K}}$. The word 'complete' here means that the knowledge of their values uniquely determines the *orbit*, i.e., the point in $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$ corresponding to the point in $e^{\mathcal{L}}$. There are $m = \dim(\mathcal{P})$ coordinates, as this is the dimension of $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$ (cf. (5)). Once we have coordinates $\{x^1, ..., x^m\}$, the corresponding tangent vectors $\{\frac{\partial}{\partial x^1}, ..., \frac{\partial}{\partial x^m}\}$ at every regular point in the quotient space determine a basis of the tangent space of $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$. For any trajectory Γ in $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$, we can write the tangent vector $\dot{\Gamma}(t)$ as $\dot{\Gamma}(t) = \sum_{j=1}^{m} \dot{x}^j \frac{\partial}{\partial x^j}$, for some functions $\dot{x}^j = \dot{x}^j(t)$. With this choice of coordinates, one then needs to calculate, for every regular point U, the matrix for $\pi_*|_U$ as restricted to $R_{U*}\mathcal{P}$ and its inverse $\pi_*|_U^{-1}$. This allows us to implement formula (7) to obtain the control from a given prescribed trajectory in the orbit space.

Once this information is available, a smooth control can be obtained. Let us first assume that the desired final condition U_f is in the regular part of $e^{\mathcal{L}}$. Since the regular part is open and dense in $e^{\mathcal{L}}$, this will actually allow us to drive the state arbitrarily close to any point in $e^{\mathcal{L}}$. The identity $\mathbf{1}$ is not in the regular part of $e^{\mathcal{L}}$. In fact the whole Lie group $e^{\mathcal{K}}$ is the isotropy group of the identity, so that $\mathbf{1}$ is in the singular part. If we take for Γ a trajectory which starts from the class corresponding to the identity, the matrix corresponding to π_* may become singular as $t \to 0$ and therefore it will be impossible to derive the control directly from formula (7). We cannot therefore simply prescribe a curve Γ in the quotient space joining the identity to the desired orbit. In order to overcome this problem, we apply a *preliminary* continuous *control* which takes the state of system (2) (from the identity) out of the singular part and into the regular part of $e^{\mathcal{L}}$. To avoid discontinuities, such a control is chosen to be zero at the beginning and at the end of the control interval. It takes the system to a point U_0 with $\pi(U_0) = \Gamma_0 \in e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$.

There is no general prescription to design such a preliminary control which depends on the particular system at hand. However we recall that the regular part of $e^{\mathcal{L}}/e^{\mathcal{K}}$ is *open and dense* in $e^{\mathcal{L}}/e^{\mathcal{K}}$, therefore, only special types of controls will keep the state in the singular part. An arbitrary control function will likely do the job to move the state from the identity to a point U_0 in $e^{\mathcal{L}}_{reg}$. Then we choose the trajectory Γ in the regular part of the quotient space which joins Γ_0 and Γ_1 where Γ_1 is the orbit of the desired final condition U_f. The control obtained through (7) will steer system (2) to a state $\hat{U}_f$ in the same orbit as the desired final condition U_f. Therefore we will have $\pi(\hat{U}_f) = \pi(U_f) = \Gamma_1$. Notice that we also want $\dot{\Gamma} = 0$ at both the initial and final point so that the control is zero and can be *concatenated* continuously with the preliminary control above described. The (concatenated) control $\hat{u}$ obtained this way will drive the state U of (2) from the identity $\mathbf{1}$ to a state $\hat{U}_f$ which is in the same orbit as the desired final state U_f. There exists $K \in e^{\mathcal{K}}$ such that $K\hat{U}_f K^{-1} = U_f$. Once such a K is found it will determine through $\sum_{j=1}^{m} KB_j\hat{u}_jK^{-1} = \sum_{k=1}^{m} B_k u_k$ the actual control $\{u_k\}$ to apply. Such a 'rotated' control is the final control for the procedure. We remark that this 'rotation' procedure does not modify the smoothness properties of the control, nor the fact that it is zero at some point (in particular at the beginning and at the end of the control interval).

Assume now that the desired final condition U_f is in the singular part of $e^{\mathcal{L}}$. The problem is solved by concatenating two controls which drive the identity to two regular points obtained as described above. In particular, we first select a regular element $S \in e^{\mathcal{L}}$ and such that $U_f S^{-1}$ is also regular [3]. Then we find two controls: u_1 driving U in (2) from the identity to S in (2) and u_2 driving U in (2) from the identity to $U_f S^{-1}$ in (2). Because of the right invariance of system (2), u_2 also drives S to U_f. Therefore, the concatenation of u_1 (first) and u_2 (second) will drive to the desired final state U_f.

2.4 Examples

2.4.1 Control of a single spin $\frac{1}{2}$ particle

Consider the Schrödinger operator equation (2) in the form

$$\dot{U} = \begin{pmatrix} 0 & \alpha(t) \\ -\alpha^*(t) & 0 \end{pmatrix} U, \qquad U(0) = \mathbf{1}_2, \tag{8}$$

with U in $SU(2)$. The complex-valued function α is a complex control field representing the x and y components of an electro-magnetic field. The dynamical Lie algebra $\mathcal{L}$ is $\mathfrak{su}(2)$ and it has a decomposition $\mathfrak{su}(2) = \mathcal{K} \oplus \mathcal{P}$ with $\mathcal{K}$ diagonal and $\mathcal{P}$ anti-diagonal matrices. The one-dimensional Lie group of *diagonal* matrices in $SU(2) = e^{\mathcal{L}}$ is a symmetry group $e^{\mathcal{K}}$ for the above system and the structure of the quotient space $SU(2)/e^{\mathcal{K}}$ is that of a closed unit disc [11]. The entry $u_{1,1}$ of $U \in SU(2)$, which is a complex number with absolute value ≤ 1, determines the orbit of the matrix U. The regular part of $SU(2)$ corresponds to matrices with $|u_{1,1}| < 1$, i.e., the interior of the unit disc, in the complex plane. The singular part is the boundary of the unit disc. Denote by z the (complex) coordinate in the interior of the complex unit disc. This corresponds to two *real* coordinates invariant under the action of $e^{\mathcal{K}}$ (conjugation by diagonal matrices). Let $\Gamma = \Gamma(t)$ be a desired trajectory inside the unit disc, which we denote by z_d in the chosen coordinates. The tangent vector $\dot{\Gamma}$ in (6) is given in the complex coordinate by $\dot{z}_d \frac{\partial}{\partial z}$. (This is a shorthand notation for $\dot{x}_d \frac{\partial}{\partial x_d} + \dot{y}_d \frac{\partial}{\partial y_d}$ where x_d and y_d are the real and imaginary parts of z_d.) In the coordinates on $SU(2)$ used in equation (2) the corresponding tangent vector for $\dot{U}$ is given by (cf. (8)) $\begin{pmatrix} 0 & \alpha \\ -\alpha & 0 \end{pmatrix} U$

and the value of the control α is obtained by solving (6) which becomes in this case:

$$\dot{z}_d = \frac{d}{dt}|_{t=0} z \left(e^{\begin{pmatrix} 0 & \alpha \\ -\alpha^* & 0 \end{pmatrix} t} U \right), \tag{9}$$

where $z(P)$ denotes the the $(1,1)$ entry of the matrix P. Equation (9) gives $\alpha = \frac{\dot{z}_d}{u_{2,1}}$, which, as expected from the above recalled isomorphism theorem of [18], gives a one-to-one correspondence between α and $\dot{z}_d$ as long as U is in the regular part of $SU(2)$, i.e., it is not diagonal, i.e., $u_{2,1} \neq 0$.

The right hand side of (2) in this case takes the form $u_x i\sigma_x + u_y i\sigma_y$, with $\sigma_{x,y,z}$ the Pauli matrices defined in (19) below, so that α above is $\alpha := u_y + iu_x$. Writing $u_{2,1} := u + iv$, equation (9) gives the controls in terms of the desired trajectory in the quotient space $(\dot{x}_d,\, \dot{y}_d)$ as $u_y = \frac{u\dot{x}_d + v\dot{y}_d}{u^2+v^2}$, $u_x = \frac{u\dot{y}_d - v\dot{x}_d}{u^2+v^2}$.

As a numerical example, assume we want to steer the state from the identity $\mathbf{1}_2$ to $U_f = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$. Notice that the desired final value U_f is in the singular part of the space. Therefore, as described in the previous subsection, we split the problem in two: we drive to a regular S (such that $U_f S^{-1}$ is also regular) and to $U_f S^{-1}$ and then concatenate the two controls. We first apply a preliminary control to move the state out of the singular part. To do that, we can use in an interval $[0,1]$ $u_x \equiv 0$ and u_y any function such that $\int_0^1 u_y(t) = \frac{\pi}{4}$, and $u_y(0) = 0$ and $u_y(1) = 0$, for example $u_y(t) = \frac{\pi^2}{8}\sin(\pi t)$. This drives the state to the intermediate value $U_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$. Call the corresponding control u_1. We notice that U_1 is a regular point, and

$$U_f U_1^{-1} = \begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \end{pmatrix}, \tag{10}$$

is also a regular point, and therefore we can take U_1 as the regular intermediate point S and the problem is now to find a control which drives the identity to $U_f S^{-1} = U_f U_1^{-1}$ in (10). Then we concatenate the control that drives to S, i.e., u_1, with the one that drives to $U_f S^{-1}$ to obtain a (smooth) control that drives to U_f. Again, apply a preliminary control driving the state from the identity out of the singular part. Similarly as before we can use, in an interval $[0,1]$, $u_x \equiv 0$ and $u_y = \hat{u}_y$ any function such that $\int_0^1 u_y(t) = \frac{\pi}{4}$, $u_y(0) = 0$ and $u_y(1) = 0$, so that we drive to $U_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. Note that there is no special reason here to change the intermediate point in the regular part different from the one before. We only want to avoid confusion between the two steps, and our choice makes things slightly simpler in the following calculations. Now consider a trajectory (x_d, y_d) in the quotient space (the disk) from the point 0 to the point $\frac{i}{\sqrt{2}} = \pi(U_f S^{-1})$ (cf. (10)), such that at the initial and final time $\dot{x}_d = \dot{y}_d = 0$. We can choose for example, in $[0,1]$, the polynomials $x_d(t) \equiv 0$, $y_d(t) = \frac{t^2}{\sqrt{2}}(3-2t)$. With this choice, $\dot{x}_d \equiv 0$ and $\dot{y}_d = \frac{6}{\sqrt{2}}t(1-t)$, and the controls $u_x = \frac{u\dot{y}_d - v\dot{x}_d}{u^2+v^2}$ and $u_y = \frac{u\dot{x}_d + v\dot{y}_d}{u^2+v^2}$ become:

$$u_x = \frac{\frac{6t}{\sqrt{2}}(1-t)u}{u^2+v^2}, \qquad u_y = \frac{\frac{6t}{\sqrt{2}}(1-t)v}{u^2+v^2},$$

which gives $\alpha := i\frac{6t(1-t)}{\sqrt{2}\|u_{2,1}\|^2}u_{2,1}^*$. Then we solve the differential system

$$\dot{u}_{1,1} = \alpha u_{2,1}; \qquad \dot{u}_{2,1} = -\alpha^* u_{1,1} \qquad [u_{1,1}(0), u_{2,1}(0)] = [0,-1].$$

This step is usually done numerically but, in this case, we can obtain an explicit solution which is given by:

$$u_{1,1}(t) = \frac{i}{\sqrt{2}}(3t^2 - 2t^3), \qquad u_{2,1} = -\sqrt{1 + 2(-t^6 + 3t^5 - \frac{9}{4}t^4)}. \tag{11}$$

The controls u_x and u_y are:

$$u_x = -\frac{6t(1-t)}{\sqrt{2}\sqrt{1 + 2(-t^6 + 3t^5 - \frac{9}{4}t^4)}}, \qquad u_y \equiv 0 \tag{12}$$

which have to be 'concatenated' to the control, $u_x \equiv 0, u_y = \hat{u}_y$ that drives to U_2. Such a concatenated control leads to $\hat{U}_f = \begin{pmatrix} \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \end{pmatrix}$ (calculated by using $t = 1$ in (11)). This is different from the desired $U_f U_1^{-1} = U_f S^{-1}$ in (10), but in the same orbit. The transformation $K \in e^{\mathcal{K}}$, $K := \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix}$, with $\phi = \frac{\pi}{4}$ is such that $K\hat{U}_f K^\dagger = U_f S^{-1}$. Therefore the control to reach $U_f S^{-1}$ is the above (concatenated) control steering to $\hat{U}_f$ 'rotated' by K. In particular, consider the control u_x, u_y above which is the concatenation of $u_x \equiv 0, u_y = \hat{u}_y$ and (u_x, u_y) in (12). Consider $K(u_y i\sigma_y + u_x i\sigma_x)K^\dagger = u_y K i\sigma_y K^\dagger + u_x K i\sigma_x K^\dagger = u_y i\sigma_x - u_x i\sigma_y$. Therefore the new control is such that the role of u_x is taken by the old u_y and the role of u_y is taken by $-$ the old u_x. This control drives the state from the identity to $U_f S^{-1}$. Concatenating this control with the control leading to S gives a control steering to the desired final condition U_f.

2.4.2 Control of a three level system in the Λ configuration

Consider a three level quantum system where the controls couple level $|1\rangle$ to level $|2\rangle$ and level $|1\rangle$ to level $|3\rangle$ but not level $|2\rangle$ and $|3\rangle$ directly. Assuming that $|1\rangle$ is the highest energy level, the energy level diagram takes the so-called Λ configuration (see, e.g., [25]). The Schrödinger operator equation (2) is such that

$$\sum_{j=1}^{m} u_j B_j = \sum_{j=1}^{4} u_j B_j = \begin{pmatrix} 0 & \alpha & \beta \\ -\alpha^* & 0 & 0 \\ -\beta^* & 0 & 0 \end{pmatrix}, \tag{13}$$

with the complex control functions α and β. Such a system admits a group of symmetries given by $e^{\mathcal{K}} = S(U(1) \times U(2))$, i.e., block diagonal matrices in $SU(3)$ with one block of dimension 1×1 and one block of dimension 2×2, and determinant equal to 1. The Lie subalgebra $\mathcal{K}$ consists of matrices in $\mathfrak{su}(3)$ with a block diagonal structure with one block of dimension 1×1 and one block of dimension 2×2. The complementary subspace $\mathcal{P}$ is spanned by antidiagonal matrices in $\mathfrak{su}(2)$ with the same partition of rows and columns. Such a system was studied in [12] in the context of optimal control and a description of the orbit space $SU(3)/e^{\mathcal{K}}$ was given there. It was shown that the regular part $SU(3)_{reg}/e^{\mathcal{K}}$ is homeomorphic to the product of two open unit discs $\mathring{D}_1 \times \mathring{D}_2$ in the complex plane. Up to a similarity transformation in $e^{\mathcal{K}} = S(U(1) \times U(2))$, a matrix U in $SU(3)$ can be written as

$$U = \begin{pmatrix} z_1 & \sqrt{1-|z_1|^2} & 0 \\ -\sqrt{1-|z_1|^2} & z_1^* & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & z_2 & w \\ 0 & -w^* & z_2^* \end{pmatrix}, \tag{14}$$

for complex numbers z_1, z_2 and w, where $|z_1| \leq 1$ and $|z_2| \leq 1$. Strict inequalities hold if and only if U is in the regular part, in which case z_1 and z_2 can be taken as the coordinates in $SU(3)_{reg}/e^{\mathcal{K}}$. An alternative set of (complex) coordinates is given by (z_1, T) where T is the trace of the (lower) 2×2 block of $U \in SU(3)$

which is invariant (along with z_1) under the conjugation action of elements in $e^{\mathcal{K}} = S(U(1)\times U(2))$. The coordinates (z_1, T) are related to the coordinates (z_1, z_2) (from (14)) by $T = z_1^* z_2 + z_2^*$ which is inverted as $z_2 = \frac{T^* - z_1 T}{1-|z_1|^2}$. A (desired) trajectory Γ in $SU(3)_{reg}/S(U(1)\times U(2))$ is written in these coordinates as $(z_{1d}, T_d) := (z_{1d}(t), T_d(t))$. The associated tangent vector $\dot{\Gamma}$ in (6) is $\dot{z}_{1d}(t)\frac{\partial}{\partial z_1} + \dot{T}_d\frac{\partial}{\partial T}$. By using (6) with the restriction that $\dot{U}$ is of the form $\begin{pmatrix} 0 & \alpha & \beta \\ -\alpha^* & 0 & 0 \\ -\beta^* & 0 & 0 \end{pmatrix} U$, we obtain two equations for α and β,

$$\alpha u_{2,1} + \beta u_{3,1} = \dot{z}_{1d}, \qquad -\alpha u_{1,2}^* - \beta u_{1,3}^* = \dot{T}_d^*.$$

These are solved, using $\hat{D} := u_{1,3}^* u_{2,1} - u_{3,1} u_{1,2}^*$ by

$$\alpha = \frac{u_{1,3}^* \dot{z}_{1,d} + u_{3,1}\dot{T}_d^*}{\hat{D}}, \qquad \beta = -\frac{u_{1,2}^* \dot{z}_{1,d} + u_{2,1}\dot{T}_d^*}{\hat{D}}. \tag{15}$$

The quantity $\hat{D}$ is different from zero if and only if the matrix U is in the regular part of $SU(3)$ [4].

We illustrate the procedure for this system with a numerical example. Assume our desired final condition is

$$U_f := \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -1 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{16}$$

The invariant coordinates are $z_1 = 0$ and $T = \frac{1}{\sqrt{2}}$ which gives $z_2 = \frac{1}{\sqrt{2}}$. Since $|z_1| < 1$, $|z_2| < 1$ the desired final condition is in the regular part of the space. We need to apply a preliminary control to steer the state away from the identity. We use for this control a sequence $u_2 \circ u_1$ where, for u_1 (u_2), $\alpha \equiv 0$ $(\beta \equiv 0)$ and β (α) is any real continuous function which is zero at the endpoints of the interval and whose integral in the interval is $\frac{\pi}{2}$. This control drives the state to $U_1 := \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}$, which is in the regular part with $z_1 = z_2 = T = 0$. Therefore, in the quotient space, we look for a (smooth) trajectory (z_{1d}, T_d) connecting $(z_1, T) = (0, 0)$ to $(z_1, T) = (0, \frac{1}{\sqrt{2}})$. We can take in $[0, 1]$, $z_{1d} \equiv 0$, $T_d = -\sqrt{2}t^3 + \frac{3}{\sqrt{2}}t^2$. With this choice, α and β in (15) are given by

$$\alpha = \frac{3\sqrt{2}t(1-t)u_{3,1}}{u_{1,3}^* u_{2,1} - u_{3,1}u_{1,2}^*}, \qquad \beta = -\frac{3\sqrt{2}tu_{2,1}}{u_{1,3}^* u_{2,1} - u_{3,1}u_{1,2}^*}. \tag{17}$$

With these controls we integrate the Schrödinger equation (2), (13) of the system with initial condition U_1. From the numerical solution of this differential system, we obtain the explicit form of the controls $\alpha = \alpha(t)$ and $\beta = \beta(t)$ as well as the final condition which turns out to be

$$\hat{U}_f = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -1 & 0 & 0 \end{pmatrix}.$$

This, as expected, is in the same orbit as the desired final condition U_f in (16). The matrix $K := \begin{pmatrix} e^{\frac{i\pi}{3}} & 0 & 0 \\ 0 & 0 & e^{\frac{i\pi}{3}} \\ 0 & e^{\frac{i\pi}{3}} & 0 \end{pmatrix} \in e^{\mathcal{K}}$ is such that $K\hat{U}_f K^\dagger = U_f$. Therefore the control is the concatenation of the preliminary one (used to drive the state away from the identity and into the regular part, i.e., to U_1) and the (α, β) obtained by the above numerical integration, everything rotated by the matrix K.

3 Simultaneous control of two independent spin $\frac{1}{2}$ particles

3.1 The model

The dynamics of two spin $\frac{1}{2}$ particles with different gyromagnetic ratios in zero field NMR can be described by the Schrödinger equation (2) (after appropriate normalization) where

$$\sum_{k=1}^{m} \hat{u}_k B_k := \sum_{x,y,z} u_{x,y,z}(t)(i\sigma_{x,y,z} \otimes \mathbf{1} + \gamma i \mathbf{1} \otimes \sigma_{x,y,z}). \tag{18}$$

Here $u_{x,y,z}$ are the controls representing the x, y, z components of the electromagnetic field, and $\sigma_{x,y,z}$ are the Pauli matrices defined as

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{19}$$

The parameter γ is the ratio of the two gyromagnetic ratios and we shall assume that $|\gamma| \neq 1$. Under this assumption, the dynamical Lie algebra $\mathcal{L}$ for system (2), (18) is the 6−dimensional Lie algebra spanned by $\{\sigma_1 \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_2 \,|\, \sigma_1, \sigma_2 \in \mathfrak{su}(2)\}$ [5]. The corresponding Lie group $e^{\mathcal{L}}$, which is the set of reachable states for system (2), (18), is $\{X_1 \otimes X_2 \,|\, X_1, X_2 \in SU(2)\}$, i.e. the tensor product $SU(2) \otimes SU(2)$. It is convenient to slightly relax the description of the state space and look at system (2), (18) as a system on the Lie group $SU(2) \times SU(2)$, i.e., the Cartesian direct product of $SU(2)$ with itself, and the dynamical equations (2), (18) replaced by

$$\dot{U} = \sigma(t)U, \quad U(0) = \mathbf{1}, \qquad \dot{V} = \gamma\sigma(t)V, \quad V(0) = \mathbf{1}, \tag{20}$$

with $\sigma(t) := \sum_{x,y,z} i u_{x,y,z}(t)\sigma_{x,y,z}$. The controls that drive system (20) to $(\pm U_f, \pm V_f)$ drive system (2), (18) to the state $U_f \otimes V_f$. Therefore we shall focus on the steering problem for system (20) which consists of steering one spin to U_f and the other to V_f, simultaneously. Since $|\gamma| \neq 1$, the dynamical Lie algebra associated with (20) is spanned by the pairs (σ_1, σ_2) with σ_1 and σ_2 in $\mathfrak{su}(2)$. Such a Lie algebra can be written as $\mathcal{K} \oplus \mathcal{P}$ with $\mathcal{K}$ spanned by elements of the form (σ, σ) with $\sigma \in \mathfrak{su}(2)$ and $\mathcal{P}$ spanned by elements of the form $(\sigma, \gamma\sigma)$ with $\sigma \in \mathfrak{su}(2)$. At every $p \in G = SU(2) \times SU(2)$, the vector fields in (20) belong to $R_{p*}\mathcal{P}$.

3.2 Symmetries and the the structure of the quotient space

The Lie group $SU(2)$ acts on $G := SU(2) \times SU(2)$ by *simultaneous conjugation*, that is, for $K \in SU(2)$, $(U_f, V_f) \to (KU_fK^{-1}, KV_fK^{-1})$ and this is a group of symmetries for system (20) in that if $\sigma = \sigma(t)$ is the control steering to (U_f, V_f), then $K\sigma K^{-1}$ is the control steering to (KU_fK^{-1}, KV_fK^{-1}). The quotient space of $SU(2) \times SU(2)$ under this action, $(SU(2) \times SU(2))/SU(2)$ was described in [20] as follows.

Consider a pair (U_f, V_f) and let $\phi \in [0, \pi]$ be a real number so that the two eigenvalues of U_f are $e^{i\phi}$ and $e^{-i\phi}$. If $0 < \phi < \pi$ then $U_f \neq \pm\mathbf{1}$ and there exists a unitary matrix S such that $SU_fS^\dagger := D_f$ is diagonal. Therefore the matrix (U_f, V_f) is in the same orbit as $(D_f, SV_fS^\dagger)$. The parameter ϕ determines the orbit, along with the $(1,1)-$entry of $SV_fS^\dagger$, which does not depend on the choice of S. (All the possible diagonalizing matrices differ by a diagonal factor that does not affect the $(1,1)$ entry of $SV_fS^\dagger$.) Such a $(1,1)$-entry has absolute value ≤ 1 and therefore it is an element of the unit disk in the complex plane. The orbits corresponding to the values of $0 < \phi < \pi$ (for the eigenvalue of the first matrix) are therefore in one-to-one correspondence with the points of a solid cylinder with height equal to π. When $\phi = 0$ (or $\phi = \pi$), the matrix U_f is $\pm$ identity and therefore the equivalence class is determined by the eigenvalue of the matrices V_f, which are $e^{\pm i\psi}$ for $\psi \in [0,\pi]$. In the geometric description, the solid cylinder degenerates at the two ends to become a segment $[0,\pi]$. The regular part of the orbit space G_{reg} is represented by points in the interior of the solid cylinder. Such points correspond to pairs

$$\left(\begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-i\phi} \end{pmatrix}, \begin{pmatrix} z & w \\ -w^* & z^* \end{pmatrix}\right)$$

with $\phi \in (0,\pi)$ and $|z| < 1$. For these pairs, the isotropy group is the discrete group $\{\pm\mathbf{1}\}$. In general points that are in the singular part correspond to pairs of matrices (U_f, V_f) which can be simultaneously diagonalized. Therefore the condition that they commute

$$U_f V_f = V_f U_f, \tag{21}$$

is necessary and sufficient for a pair (U_f, V_f) to belong to the singular part.

Assume that p is a regular point in G_{reg} for this problem and π is the natural projection $\pi : G_{reg} \to G_{reg}/SU(2)$. Then from the theory in the previous section, the differential $\pi_*|_p$ is an isomorphism from $R_{p*}\mathcal{P}$ to $T_{\pi(p)}G_{reg}/SU(2)$. Let us choose a basis for $\mathcal{P}$ given by $(i\sigma_{x,y,z}, \gamma i\sigma_{x,y,z})$. To choose the three coordinates in $G_{reg}/SU(2)$, we consider a general element p in $SU(2) \times SU(2)$ written as

$$p := (U_f, V_f) := \left(\begin{pmatrix} x & y \\ -y^* & x^* \end{pmatrix}, \begin{pmatrix} z & w \\ -w^* & z^* \end{pmatrix}\right). \tag{22}$$

For a complex number q we shall denoted by $q_R := \mathtt{Re}(q)$ and $q_I := \mathtt{Im}(q)$. Notice that in (22) we have

$$x_R^2 + x_I^2 + y_R^2 + y_I^2 = z_R^2 + z_I^2 + w_R^2 + w_I^2 = 1.$$

Coordinates in $G_{reg}/SU(2)$ must be independent invariant functions of (U_f, V_f) in (22). We choose

$$x^1 := x_R, \qquad x^2 := z_R, \qquad x^3 := x_I z_I + w_R y_R + w_I y_I. \tag{23}$$

It is a direct verification to check that at any point $p \in SU(2) \times SU(2)$, x^1, x^2 and x^3 are unchanged by the (double conjugation) action of $SU(2)$, i.e., they are invariant. We remark also that we can define two unit vectors $\vec{V} := (x_R, x_I, y_R, y_I)$, and $\vec{W} := (z_R, z_I, w_R, w_I)$, and, if we do that, $x^3 = \vec{V} \cdot \vec{W} - x_R z_R$.

3.3 Choice of invariants

We pause a moment to detail how the invariant coordinates in (23) were chosen. We do this because the method can be used for other examples. We consider the vectors $\vec{V} := [x_R, x_I, y_R, y_I]^T$ and $\vec{W} := [z_R, z_I, w_R, w_I]^T$ and the adjoint action of $SU(2)$ on $SU(2) \times SU(2)$ which gives a linear action on $\vec{Q} := [\vec{V}^T, \vec{W}^T]^T$. We are looking for functions $f = f(\vec{V}, \vec{W})$ invariant under this action. Given that every element of $SU(2)$ can be written according to Euler's decomposition as $e^{i\sigma_z \alpha} e^{i\sigma_y \theta} e^{i\sigma_z \beta}$, for real parameters α, β and θ, it is enough that f is invariant with respect to transformations of the form $e^{i\sigma_z \beta}$ and $e^{i\sigma_y \theta}$, for general real β and θ, in order for f to be invariant with respect to all of $SU(2)$. If $X_z := X_z(\beta) := e^{i\sigma_z \beta}$ then Ad_{X_z} acting on $[\vec{V}^T, \vec{W}^T]^T$ is

$$Ad_{X_z(\beta)} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos(\beta) & -\sin(\beta) \\ 0 & 0 & \sin(\beta) & \cos(\beta) \end{pmatrix}. \tag{24}$$

If $X_y := X_y(\theta) := e^{i\sigma_y \theta}$ then Ad_{X_y} acting on $[\vec{V}^T, \vec{W}^T]^T$ is

$$Ad_{X_y(\theta)} := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & 0 & \cos(\theta) \\ 0 & 0 & 1 & 0 \\ 0 & -\sin(\theta) & 0 & \cos(\theta) \end{pmatrix}. \tag{25}$$

We first look for *linear invariants*, i.e., invariant functions f of the form $f(\vec{V}, \vec{W}) := \vec{a}^T \vec{V} + \vec{b}^T \vec{W}$. From the condition

$$\vec{a}^T \vec{V} + \vec{b}^T \vec{W} = \vec{a}^T Ad_X \vec{V} + \vec{b}^T Ad_X \vec{W},$$

where X may be equal to $X_z(\beta)$ or $X_y(\theta)$, with arbitrary β and θ, we find that the last three components of $\vec{a}$ and $\vec{b}$ must be zero. Therefore all linear invariants f must be of the form $f = a_1 x_R + b_1 z_R$, from which we get the invariant x_R and z_R in (23).

We then try to find *quadratic invariants* and therefore an 8×8 symmetric matrix P so that $f(\vec{V}, \vec{W}) = [\vec{V}^T, \vec{W}^T] P [\vec{V}^T, \vec{W}^T]^T$ and

$$[\vec{V}^T, \vec{W}^T] P [\vec{V}^T, \vec{W}^T]^T = [\vec{V}^T, \vec{W}^T] \begin{pmatrix} Ad_X^T & 0 \\ 0 & Ad_X^T \end{pmatrix} P \begin{pmatrix} Ad_X & 0 \\ 0 & Ad_X \end{pmatrix} [\vec{V}^T, \vec{W}^T]^T,$$

for $X = X_z(\beta)$ and $X = X_y(\theta)$ as defined in (24) and (25) for every β and θ (and for every $\vec{V}$ and $\vec{W}$). This leads to the condition

$$\begin{pmatrix} Ad_X & 0 \\ 0 & Ad_X \end{pmatrix} P = P \begin{pmatrix} Ad_X & 0 \\ 0 & Ad_X \end{pmatrix}.$$

From this, we find that the matrix P must be of the form

$$P = \begin{pmatrix} e & 0 & 0 & 0 & d & 0 & 0 & 0 \\ 0 & c & 0 & 0 & 0 & g & 0 & 0 \\ 0 & 0 & c & 0 & 0 & 0 & g & 0 \\ 0 & 0 & 0 & c & 0 & 0 & 0 & g \\ d & 0 & 0 & 0 & r & 0 & 0 & 0 \\ 0 & g & 0 & 0 & 0 & h & 0 & 0 \\ 0 & 0 & g & 0 & 0 & 0 & h & 0 \\ 0 & 0 & 0 & g & 0 & 0 & 0 & h \end{pmatrix}.$$

It follows that all quadratic invariants must be of the form

$$f = e x_R^2 + 2d x_R z_R + r z_R^2 + c(x_I^2 + y_R^2 + y_I^2) + h(z_I^2 + w_R^2 + w_I^2) + 2g(x_I z_I + w_R y_R + w_I y_I).$$

Because of $x_R^2 + x_I^2 + y_R^2 + y_I^2 = z_R^2 + z_I^2 + w_R^2 + w_I^2 = 1$, all terms can be written in terms of the (linear) invariant x_R and z_R except the last one which we choose as the third coordinate in (23).

3.4 Algorithm for control

At the point $\pi(p) \in G_{reg}/SU(2)$, the tangent vectors $\frac{\partial}{\partial x^j}$, $j = 1, 2, 3$ span $T_{\pi(p)} G_{reg}/SU(2)$, so that a general tangent vector at $\pi(p)$ can be written as $a_1 \frac{\partial}{\partial x^1} + a_2 \frac{\partial}{\partial x^2} + a_3 \frac{\partial}{\partial x^3}$. We calculate the matrix of the isomorphism $\pi_*|_p$ mapping the coordinates $\alpha_x, \alpha_y, \alpha_z$, in $R_{p*}(\sigma, \gamma\sigma) := R_{p*}(\alpha_x(i\sigma_x, \gamma i \sigma_x) + \alpha_y(i\sigma_y, \gamma i \sigma_y) + \alpha_z(i\sigma_z, \gamma i \sigma_z)) \in R_{p*}\mathcal{P}$ to (a_1, a_2, a_3), (cf. (6)) to $a_1 \frac{\partial}{\partial x^1} + a_2 \frac{\partial}{\partial x^2} + a_3 \frac{\partial}{\partial x^3}$. Denote this matrix by $\Pi_{j,l} := \Pi_{j,l}(p)$ with $j = 1, 2, 3$ and $l = x, y, z$. We have

$$\Pi_{j,l}(p) = \pi_*|_p R_{p*}(i\sigma_l, i\gamma\sigma_l) x^j.$$

For the sake of illustration, let us calculate $\Pi_{1,x}(p)$. This is given by (recall p is defined in (22))

$$\Pi_{1,x}(p) := \pi_{p*}R_{p*}(i\sigma_x, i\gamma\sigma_x)x^1 = R_{p*}(i\sigma_x, i\gamma\sigma_x)(x^1 \circ \pi) = \frac{d}{dt}|_{t=0} x^1 \circ \pi \left(e^{i\sigma_x t} \begin{pmatrix} x & y \\ -y^* & x^* \end{pmatrix}, e^{i\gamma\sigma_x t} \begin{pmatrix} z & w \\ -w^* & w^* \end{pmatrix} \right).$$

This simplifies because $x^1 \circ \pi$ does not depend on the second factor. Therefore the $\Pi_{1,x}(p)$ entry is the derivative at $t = 0$ of the real part of the $(1,1)$ entry of the matrix

$$e^{i\sigma_x t} \begin{pmatrix} x & y \\ -y^* & x^* \end{pmatrix} = \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix} \begin{pmatrix} x & y \\ -y^* & x^* \end{pmatrix}.$$

This leads to the result

$$\Pi_{1,x}(p) = -y_I.$$

The quantities

$$\Delta_1 := z_I y_R - x_I w_R, \qquad \Delta_2 := z_I y_I - x_I w_I, \qquad \Delta_3 := w_R y_I - w_I y_R, \tag{26}$$

appear routinely in calculations that follow.

Similar calculations to the ones above for $\Pi_{1,x}(p)$ lead to the full matrix $\Pi(p)$, which is given by

$$\Pi(p) := \begin{pmatrix} -y_I & -y_R & -x_I \\ -\gamma w_I & -\gamma w_R & -\gamma z_I \\ (\gamma-1)\Delta_1 + \gamma z_R y_I + w_I x_R & (1-\gamma)\Delta_2 + w_R x_R + \gamma z_R y_R & (\gamma-1)\Delta_3 + x_R z_I + \gamma z_R x_I \end{pmatrix} \tag{27}$$

The determinant of this matrix is different from zero if and only if p is in the regular part and it is another invariant under the action of $SU(2)$ on $SU(2) \times SU(2)$ (cf. Appendix B). It can be explicitly computed as

$$\det(\Pi(p)) = \gamma(\gamma-1)(\Delta_1^2 + \Delta_2^2 + \Delta_3^2), \tag{28}$$

which can be seen to be equal to zero if and only if condition (21) is verified. The invariant $\Delta := \Delta_1^2 + \Delta_2^2 + \Delta_3^2$ can be expressed in terms of the (minimal) invariants x_R, z_R and x^3 in (23) as [6]:

$$\Delta = \Delta_1^2 + \Delta_2^2 + \Delta_3^2 = (1 - x_R^2)(1 - z_R^2) - (x^3)^2. \tag{29}$$

When we design a control law, the components a_1, a_2, a_3 of the tangent vector at every time t in the tangent space at $\pi(p(t))$ are given by the derivatives $\dot{x}^1$, $\dot{x}^2$, $\dot{x}^3$ of the desired trajectory in the quotient space. The corresponding components, α_x, α_y and α_z, of the tangent vector in $R_{p(t)*}\mathcal{P}$ give the appropriate control functions (u_x, u_y, u_z). The matrix $\Pi(p)$ in (27) gives the map from the control to the trajectory. Since we want to specify trajectories and compute the corresponding controls, we need the inverse of the matrix $\Pi(p)$ (cf. (7)). This is found from (27) to be

$$\det(\Pi(p))\Pi^{-1}(p) := \begin{pmatrix} \gamma(\gamma-1)(-w_R\Delta_3 - z_I\Delta_2) + \gamma^2 z_R\Delta_1 & (\gamma-1)(x_I\Delta_2 + y_R\Delta_3) + x_R\Delta_1 & \gamma\Delta_1 \\ \gamma(\gamma-1)(w_I\Delta_3 - z_I\Delta_1) - \gamma^2 z_R\Delta_2 & (\gamma-1)(x_I\Delta_1 - y_I\Delta_3) - x_R\Delta_2 & -\gamma\Delta_2 \\ \gamma(\gamma-1)(w_I\Delta_2 + w_R\Delta_1) + \gamma^2 z_R\Delta_3 & -(\gamma-1)(y_I\Delta_2 + y_R\Delta_1) + x_R\Delta_3 & \gamma\Delta_3 \end{pmatrix}. \tag{30}$$

We remark that $\Pi^{-1}(p)$ is not defined if we are in the singular part of the space $G = SU(2) \times SU(2)$ as the determinant of Π is zero there. This is in particular true at the beginning as the initial point $p \in SU(2) \times SU(2)$ is the identity. In order to follow a prescribed trajectory in the quotient space $G_{reg}/SU(2)$, we need therefore to apply a preliminary control to drive the state to an arbitrary point in G_{reg} and after that we shall apply the control corresponding to a prescribed trajectory in the quotient space.

The preliminary control in an interval $[0, T_1]$ to move the state from the singular part of the quotient space has to involve at least two different directions in the tangent space. In other terms, if we use $\sigma(t) = u(t)\sigma$ for some function $u = u(t)$ and a constant matrix $\sigma \in \mathfrak{su}(2)$ we remain in the singular part. To see this, notice that if $d := \int_0^{T_1} u(s)ds$, then the solution of (20) will be $(U_f, V_f) = (e^{d\sigma}, e^{\gamma d\sigma})$, a pair that satisfies the condition (21). Therefore the simplest control strategy of moving in one direction only will not work if we want to move the state from the singular part. Furthermore, we want $u_x(0) = u_y(0) = u_z(0) = 0$ and $u_x(T_1) = u_y(T_1) = u_z(T_1) = 0$ to avoid discontinuities at the initial time $t = 0$ and at the time of concatenation with the second portion of the control. We propose to prescribe a trajectory for $U = U(t)$ in (20) and, from that trajectory, to derive the control to be used in the equation for $V = V(t)$ in (20). We choose a smooth function $\delta := \delta(t)$ such that $\delta(0) = 0$ and $\delta(T_1) = \delta_0 \neq 0$, and $\dot{\delta}(0) = \dot{\delta}(T_1) = 0$. We also choose a smooth function $\epsilon := \epsilon(t)$, with $\epsilon(0) = \epsilon_0 \neq 0$ and $\epsilon(T_1) = 0$, and $\dot{\epsilon}(0) = \dot{\epsilon}(T_1) = 0$. We choose for $U = U(t)$ in (20)

$$U(t) = \begin{pmatrix} \cos(\delta(t)) & e^{i\epsilon(t)}\sin(\delta(t)) \\ -e^{-i\epsilon(t)}\sin(\delta(t)) & \cos(\delta(t)) \end{pmatrix}, \tag{31}$$

which at time T_1 gives

$$U(T_1) = \begin{pmatrix} \cos(\delta_0) & \sin(\delta_0) \\ -\sin(\delta_0) & \cos(\delta_0) \end{pmatrix}. \tag{32}$$

The corresponding control σ is $\sigma(t) = \dot{U}U^\dagger$, which is

$$\sigma(t) = \begin{pmatrix} i\dot{\epsilon}\sin^2(\delta) & \dot{\delta}e^{i\epsilon} + \frac{i}{2}\dot{\epsilon}\sin(2\delta)\, e^{i\epsilon} \\ -\dot{\delta}e^{-i\epsilon} + \frac{i}{2}\dot{\epsilon}\sin(2\delta)\, e^{-i\epsilon} & -i\dot{\epsilon}\sin^2(\delta) \end{pmatrix}. \tag{33}$$

Placing this in the second equation of (20) and integrating numerically we obtain the values for $V(T_1)$, the second component of (U, V), and therefore the values of (z_R, z_I, w_R, w_I). Using these values and the expression for (x_R, x_I, z_R, z_I) in (32), and using the formula for Δ given in (29), we obtain

$$\Delta = \Delta_1^2 + \Delta_2^2 + \Delta_3^2 = \sin^2(\delta_0)(1 - z_R^2(T_1) - w_R^2(T_1)) = \sin^2(\delta_0)(z_I^2(T_1) + w_I^2(T_1)), \tag{34}$$

which has to be different from zero in order for the state to be in the regular part.

The second portion of the control depends on the trajectory followed, $(x^1, x^2, x^3) = (x^1(t), x^2(t), x^3(t))$, and it is obtained by multiplying by Π^{-1} in (30) $(\dot{x}^1, \dot{x}^2, \dot{x}^3)$. The trajectory (x^1, x^2, x^3) is almost completely arbitrary. However it has to satisfy certain conditions which we now discuss. Let us denote the interval where the second part of the control is used by $[0, T_2]$. The initial condition $(x^1(0), x^2(0), x^3(0))$ has to agree with the one given by the previous interval of control. The final condition $(x^1(T_2), x^2(T_2), x^3(T_2))$ has to agree with the orbit of the desired final condition. Moreover, care has to be taken to make sure that the trajectory is such that Δ in (29) is never zero because this would create a singularity in $\Pi^{-1}(p)$. Furthermore we need $\dot{x}^1(0) = \dot{x}^2(0) = \dot{x}^3(0) = 0$, which gives $\sigma(0) = 0$, to ensure continuity with the control in the previous interval, and we also choose $\dot{x}^1(T_2) = \dot{x}^2(T_2) = \dot{x}^3(T_2) = 0$ to ensure that the control is switched off at the end of the procedure. Finally, the functions (x^1, x^2, x^3) have to be representative of a possible trajectory for special unitary matrices. This means that, with $\vec{V} := (x_R, x_I, y_R, y_I)^T$ and $\vec{W} := (z_R, z_I, w_R, w_I)^T$, $\|\vec{V}(t)\|^2 = \|\vec{W}(t)\|^2 = 1$, at every t. Therefore $|x_R(t)| < 1$ at every t, $|z_R(t)| < 1$, at every t (to avoid singularity), and from the Schwartz inequality $|\vec{V} \cdot \vec{W}| \leq 1$ we also must have $|x_R z_R + x^3| \leq 1$ and therefore

$$-1 - x_R z_R \leq x^3 \leq 1 - x_R z_R. \tag{35}$$

Once the functions $(\dot{x}^1, \dot{x}^2, \dot{x}^3)$ are chosen, the system to integrate numerically is (20) with (u_x, u_y, u_z) given by $\Pi^{-1}(p)(\dot{x}^1, \dot{x}^2, \dot{x}^3)^T$. By deriving (u_x, u_y, u_z) using the explicit expression of Π^{-1} given in

(30) and replacing into (20), it is possible to obtain a simplified system of differential equations for $(x_R, x_I, ..., z_R, z_I, ..., w_I)$ without implementing the preliminary step of calculating the control. We found this system to be more stable in numerical integration with MATLAB and report it in Appendix A for future use.

3.5 Numerical example: Driving to two different Hadamard gates

We now apply the above technique to a specific numerical example: The problem is to drive the system (18) so that the first spin performs the Hadamard-type gate

$$H_1 := \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \tag{36}$$

and the second spin performs the Hadamard gate

$$H_2 := \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-i}{\sqrt{2}} \\ \frac{-i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{37}$$

We want to drive system (20) to $(U_f, V_f) = (H_1, H_2)$. The orbit of the desired final condition is characterized by the invariant coordinates

$$x^1 = x_R = \frac{1}{\sqrt{2}}, \qquad x^2 = z_R = \frac{1}{\sqrt{2}}, \qquad x^3 = x_I z_I + y_R w_R + y_I w_I = 0. \tag{38}$$

We take a physical value for the ratio γ between the two gyromagnetic ratios. In particular we will choose $\gamma \approx \frac{1}{0.2514}$ which corresponds to the Hydrogen-Carbon $({}^1H - {}^{13}C)$ system also considered in [20].

We first consider the control that moves the state away from the singular part, in a time interval $[0, 1]$. We choose σ in (33) with the functions δ and ϵ as follows:

$$\delta = 6\delta_0 \left(\frac{t^2}{2} - \frac{t^3}{3} \right), \qquad \epsilon = \epsilon_0 + 6\epsilon_0 \left(\frac{t^3}{3} - \frac{t^2}{2} \right). \tag{39}$$

With these functions δ and ϵ, σ satisfies all the requirements described above. From (39) and (33) we obtain the controls u_x, u_y, u_z which replaced into (20) give the dynamics in the interval $[0, T_1] = [0, 1]$. Numerical integration with the values of the parameters $\delta_0 = 0.5$ and $\epsilon_0 = 1$, gives the following conditions at time $T_1 = 1$ (cf. (32)

$$U(1) = \begin{pmatrix} \cos(0.5) & \sin(0.5) \\ -\sin(0.5) & \cos(0.5) \end{pmatrix}, \qquad V(1) \approx \begin{pmatrix} -0.3472 + i0.7769 & -0.5123 - i0.1157 \\ 0.5123 - i0.1157 & -0.3472 - i0.7769 \end{pmatrix}. \tag{40}$$

The value of Δ is, according to (34), $\Delta \approx \sin^2(0.5) \left((0.7769)^2 + (0.1157)^2 \right) \neq 0$, as desired.

The values of the variables to be used as initial conditions in the integration in the subsequent interval of the procedure are $x_R(1) = x^1(1) = \cos(0.5)$, $x_I(1) = 0$, $y_R(1) = \sin(0.5)$, $y_I(1) = 0$, $z_R(1) = x^2(1) = -0.3472$, $z_I(1) = 0.7769$, $w_R(1) = -0.5123$, $w_I(1) = -0.1157$, and $x^3(1) = x_I(1)z_I(1) + y_R(1)w_R(1) + y_I(1)w_I(1) = \sin(0.5) \times (-0.5123) \approx -0.2456$. For the subsequent interval $[0, T_2]$ we choose the trajectory $x^1(t), x^2(t), x^3(t)$ in the quotient space as follows: $T_2 = 10$ and the trajectory in the interval $[0, T_2]$ is

$$x^1(t) = -\frac{1}{500} \left(\frac{1}{\sqrt{2}} - \cos(0.5) \right) t^3 + \frac{3}{100} \left(\frac{1}{\sqrt{2}} - \cos(0.5) \right) t^2 + \cos(0.1); \tag{41}$$

$$x^2(t) = -\frac{1}{500}\left(\frac{1}{\sqrt{2}} + 0.3472\right)t^3 + \frac{3}{100}\left(\frac{1}{\sqrt{2}} + 0.3472\right)t^2 - 0.3472; \tag{42}$$

$$x^3(t) := \frac{-0.2456}{500}t^3 - \frac{3\times(-0.2456)}{100}t^2 - 0.2456, \tag{43}$$

which are easily seen to satisfy the conditions at the endpoints. Moreover by plotting x^1 and x^2 we see that $|x^1(t)| \le 1$ and $|x^2(t)| \le 1$ for every $t \in [0, 10]$ (Figure 1). By plotting x^3 vs $1 - x^1x^2$ and $-1 - x^1x^2$ (Figure 2) we find that $-1 - x^1x^2(t) \le x^3(t) \le 1 - x^1x^2(t)$ for every $t \in [0, 10]$ as required from condition (35). By plotting $\Delta = \Delta(t)$ in $[0, 10]$ we know that $\Delta(t) \ne 0$ for every $t \in [0, 10]$ (Figure 3). Therefore the whole trajectory is in the regular part.

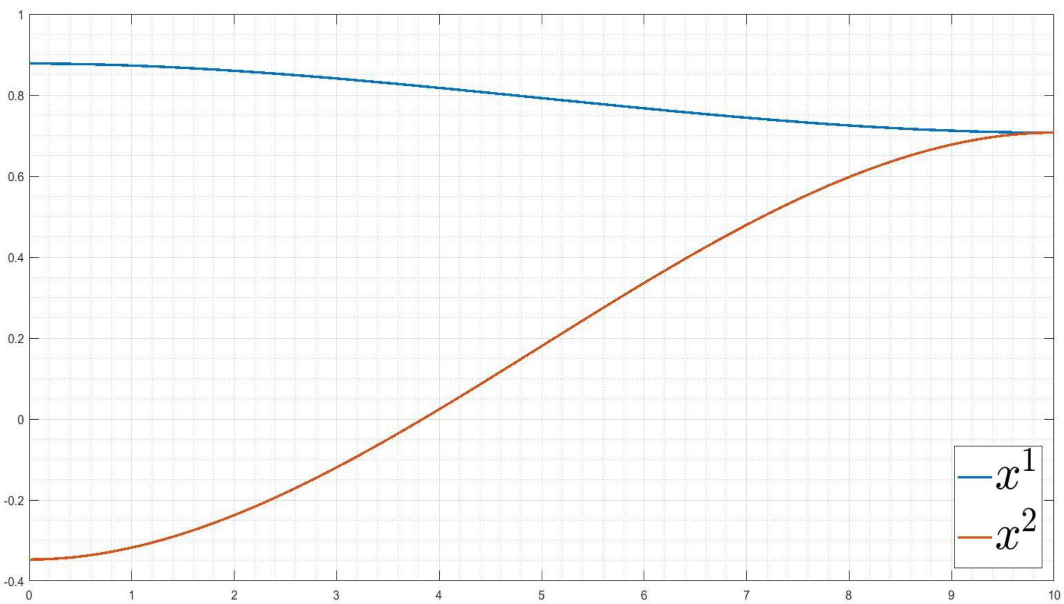

Figure 1: Prescribed x^1 and x^2 variables in the (second) interval $[0, 10]$.

The *full* trajectory, in the union of the two intervals, and with the concatenation of the two controls is depicted in Figure 4. Let us denote the full control by $\hat{\sigma} = \hat{\sigma}(t) = u_x i\sigma_x + u_y i\sigma_y + u_z i\sigma_z$. The final condition $(\hat{U}_f, \hat{V}_f)$ is given by

$$\hat{U}_f = \begin{pmatrix} 0.7071 - 0.2795i & 0.5913 + 0.2685i \\ -0.5913 + 0.2685i & 0.7071 + 0.2795i \end{pmatrix}, \qquad \hat{V}_f = \begin{pmatrix} 0.7071 + 0.2708i & 0.3718 - 0.5369i \\ -0.3718 - 0.5369i & 0.7071 - 0.2708i \end{pmatrix}. \tag{44}$$

This condition, as expected, is in the same orbit as the desired final condition (H_1, H_2) in (36), (37), that is, there exists a matrix $K \in SU(2)$ such that $K\hat{U}_f K^\dagger = H_1$ and $K\hat{V}_f K^\dagger = H_2$. The matrix K solving these equations is found to be

$$K = \begin{pmatrix} 0.1485 - 0.2460i & -0.2444 + 0.9260i \\ 0.2444 + 0.9260i & 0.1485 + 0.2460i \end{pmatrix}.$$

In particular, to find K one can diagonalize $\hat{U}_f$ and H_1, i.e., $\hat{U}_f = P\Lambda P^\dagger$ and $H_1 = R\Lambda R^\dagger$ for a diagonal matrix Λ, so that, from $KP\Lambda P^\dagger K^\dagger = R\Lambda R^\dagger$, we find that $R^\dagger K P = D$, for D, a diagonal matrix. This matrix is found by solving $DP^\dagger \hat{V}_f P = R^\dagger H_2 R D$. The control $K\hat{\sigma}K^\dagger$ steers then to the desired final condition. The resulting trajectory leading to the desired final condition (36), (37) is given in Figure 5.

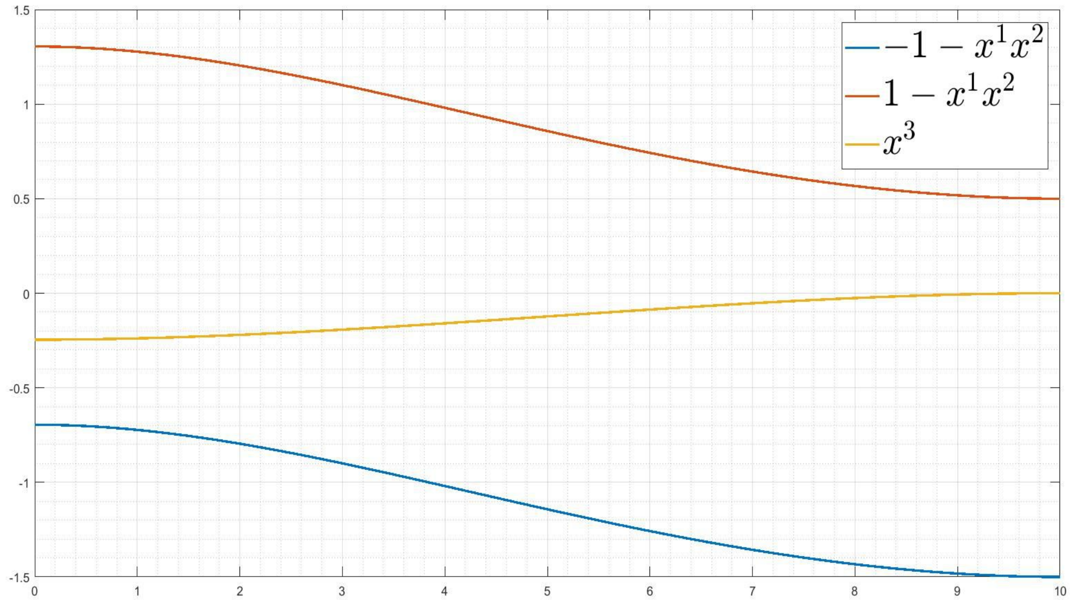

Figure 2: $x^3 = x^3(t)$ vs $-1 - x^1(t)x^2(t)$ and $1 - x^1(t)x^2(t)$ in the (second) interval $[0, 10]$.

Acknowledgment

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[1] More discussion on these basic facts in the theory of Lie transformation groups can be found in [10] and references therein.

[2] Recall that for a map $f : M \to N$ for two manifolds M and N, f_* denotes the *differential* (also called *push-forward*) $f_* : T_xM \to T_{f(x)}N$ between two tangent spaces. When we want to emphasize the point x we write $f_*|_x$.

[3] Such an element $S \in e^{\mathcal{L}}_{\text{reg}}$ always exists for any $U_f \in e^{\mathcal{L}}$, by the following argument: Assume that it does not exist. Then for every regular S, U_fS is singular (Notice that S is regular if and only if S^{-1} is regular since S and S^{-1} have the same isotropy group. Therefore we use S instead of S^{-1} in the argument). By indicating by L_U the left translation by U we have, $L_{U_f}(e^{\mathcal{L}}_{\text{reg}}) \subseteq e^{\mathcal{L}}_{\text{sing}}$. Then by applying the unique bi-invariant Haar measure μ on $e^{\mathcal{L}}$ with $\mu(e^{\mathcal{L}}) = 1$ implies $\mu(e^{\mathcal{L}}_{\text{reg}}) = \mu(L_{U_f}(e^{\mathcal{L}}_{\text{reg}})) \leq \mu(e^{\mathcal{L}}_{\text{sing}})$. On the other hand, $\mu(e^{\mathcal{L}}_{\text{sing}}) = 0$ since μ must also correspond to the Riemannian volume of the bi-invariant Killing metric (normalized if necessary) and each stratum in $e^{\mathcal{L}}_{\text{sing}}$ has dimension strictly less than dimension of $e^{\mathcal{L}}$ and thus has volume 0 and therefore invariant measure 0. But $\mu(e^{\mathcal{L}}_{\text{reg}}) = \mu(e^{\mathcal{L}}) - \mu(e^{\mathcal{L}}_{\text{sing}}) = \mu(e^{\mathcal{L}}) = 1$. This is a contradiction.

[4] This can be shown in two steps: First one shows that $\hat{D}$ is invariant under the action of $S(U(1) \times U(2))$ by writing a matrix in $S(U(1) \times U(2))$ with an Euler-type decomposition as F_1RF_2 with F_1 and F_2 diagonal and R of the form $R = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\theta) & \sin(\theta) \\ 0 & -\sin(\theta) & \cos(\theta) \end{pmatrix}$, and verifying that conjugation by each

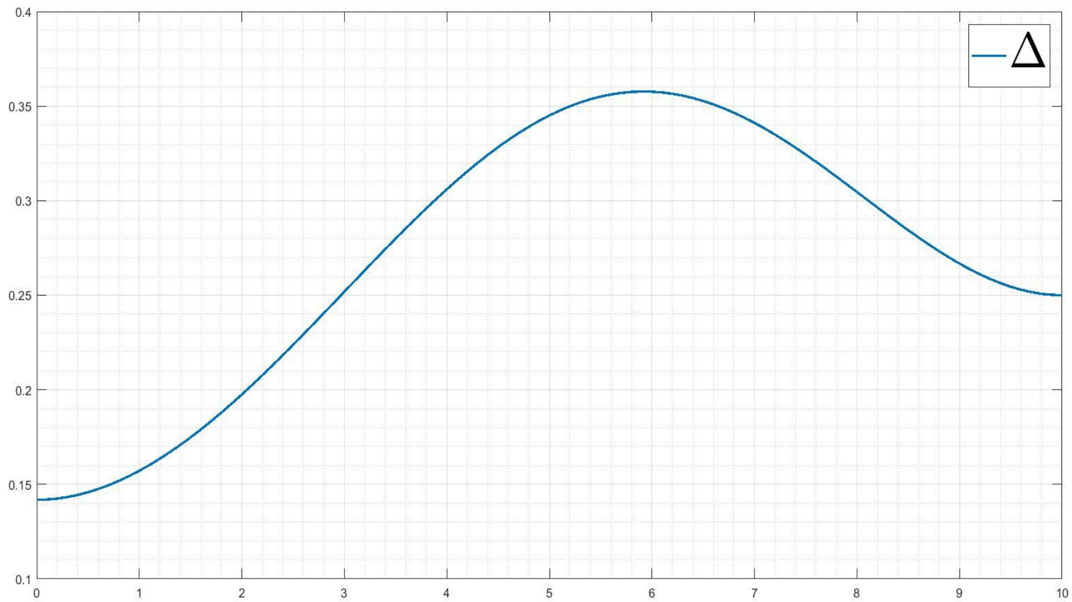

Figure 3: $\Delta = \Delta(t) = \Delta_1^2(t) + \Delta_2^2(t) + \Delta_3^2(t)$ in the (second) interval $[0, 10]$.

factor in $F_1 R F_2$ leaves $\hat{D}$ unchanged. The second step is to verify that $\hat{D}$ for the matrix X in the form (14) is different from zero if and only if $|z_1| \neq 1$ and $|z_2| \neq 1$. This gives a quick test to check whether a matrix is in the regular part, i.e., if its isotropy group is the smallest possible one, which, in this case, is the group of scalar matrices in $SU(3)$. This fact also follows from the result in Appendix B which shows in general that $\det(\pi_*)$, with $\pi_* : R_{p*}\mathcal{P} \to T_{\pi(p)} e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$ is invariant under the action of $e^{\mathcal{K}}$.

[5] This Lie algebra is isomorphic to $\mathfrak{so}(4)$.

[6] This can be seen by expanding the left hand side using the definitions of $\Delta_{1,2,3}$ (26) and the right hand side using the definition of x^3 (23), so that (29) reduces to $y_I^2 w_R^2 + w_I^2 y_R^2 + y_R^2 z_I^2 + x_I^2 w_R^2 + x_I^2 w_I^2 + y_I^2 z_I^2 = (1 - x_R^2)(1 - z_R^2) - z_I^2 x_I^2 - y_R^2 w_R^2 - y_I^2 w_I^2$, and writing $(1 - x_R^2) = x_I^2 + y_R^2 + y_I^2$ and $(1 - z_R^2) = z_I^2 + w_R^2 + w_I^2$, we obtain an identity.

[7] This follows from the definitions. For any function f, we have $\pi_* R_{p*P} f = R_{p*} P(f \circ \pi) = \frac{d}{dt}|_{t=0} f \circ \pi(e^{Pt}p) = \frac{d}{dt}|_{t=0} f \circ \pi(k e^{Pt} p k^{-1}) = \frac{d}{dt}|_{t=0} f \circ \pi(e^{kPk^{-1}t} kpk^{-1}) = \pi_* R_{kpk^{-1}} kPk^{-1}$.

[8] The fact that the matrix $\{a_s^l\}$, representing the adjoint action, is orthogonal is a consequence of the fact that the inner product, which is the Killing form on $\mathcal{P}$ is bi-invariant, and therefore it is not changed by the adjoint action.

[9] Note that $\det(A(k)) \neq -1$, since $A : e^{\mathcal{K}} \to O(m, \mathbb{R})$; $A \mapsto A(k)$ is continuous and $\det(A(k)) = \det(\mathbf{1}_m) = 1$.

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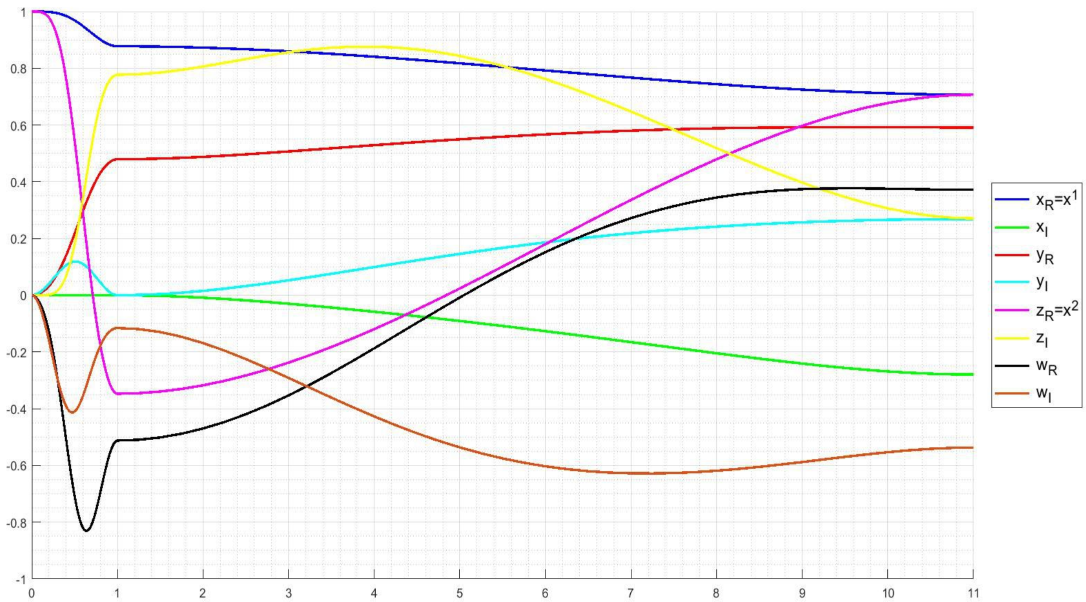

Figure 4: Trajectory under the preliminary control in the total interval $[0, 11]$.

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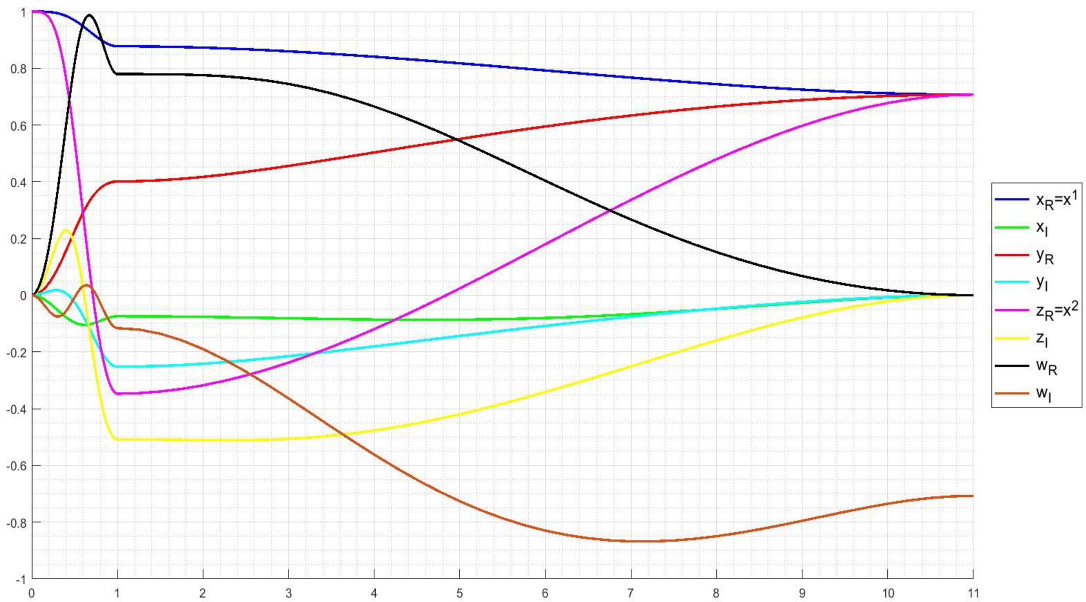

Figure 5: Trajectory under control algorithm leading to the desired final condition (36) and (37).

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4 Appendix A: System of ODE's for the simultaneous control of two quantum bits in Subsection 3.4

We derived the system of ODE's (20) with (u_x, u_y, u_z) obtained from $(u_x, u_y, u_z)^T = \Pi^{-1}(p)(\dot{x}^1, \dot{x}^2, \dot{x}^3)^T$ with Π^{-1} given in (30). We define in the following $\Delta := \Delta_1^2 + \Delta_2^2 + \Delta_3^2$, $Z := x^3 := x_I z_I + y_R w_R + y_I w_I$. Simplifications are obtained using the following two relations which are directly verified.

$$y_I \Delta_1 - y_R \Delta_2 + x_I \Delta_3 = 0,$$

$$w_I \Delta_1 - w_R \Delta_2 + z_I \Delta_3 = 0.$$

The system becomes with $a := \dot{x}^1$, $b := \dot{x}^2$, $c := \dot{x}^3$

$$\dot{x}_R = a$$
$$\gamma(\gamma-1)\Delta\dot{x}_I = (1-\gamma)\Delta_3 b + (\gamma^2 z_R a + \gamma c + \gamma b x_R)(x_R\Delta_3 - y_I\Delta_2 - y_R\Delta_1) + \gamma(\gamma-1)a(\Delta_3 Z + x_R(w_I\Delta_2 + w_R\Delta_1))$$
$$\gamma(\gamma-1)\Delta\dot{y}_R = (\gamma-1)\Delta_2 b + (\gamma^2 z_R a + \gamma c + \gamma b x_R)(x_I\Delta_1 - x_R\Delta_2 - y_I\Delta_3) + \gamma(\gamma-1)a(-\Delta_2 Z + x_R(w_I\Delta_3 - z_I\Delta_1))$$
$$\gamma(\gamma-1)\Delta\dot{y}_I = (1-\gamma)\Delta_1 b + (\gamma^2 z_R a + \gamma c + \gamma b x_R)(x_R\Delta_1 + x_I\Delta_2 + y_R\Delta_3) + \gamma(\gamma-1)a(\Delta_1 Z - x_R(w_R\Delta_3 + z_I\Delta_2))$$
$$\dot{z}_R = b$$
$$(\gamma-1)\Delta\dot{z}_I = \gamma(\gamma-1)\Delta_3 a + (\gamma z_R a + \gamma c + x_R b)(z_R\Delta_3 - w_R\Delta_1 - w_I\Delta_2) + (1-\gamma)b(\Delta_3 Z + z_R(y_R\Delta_1 + y_I\Delta_2))$$
$$(\gamma-1)\Delta\dot{w}_R = \gamma(1-\gamma)\Delta_2 a + (\gamma z_R a + \gamma c + x_R b)(z_I\Delta_1 - \Delta_3 w_I - z_R\Delta_2) + (\gamma-1)b(\Delta_2 Z + z_R(x_I\Delta_1 - y_I\Delta_3))$$
$$(\gamma-1)\Delta\dot{w}_I = \gamma(\gamma-1)\Delta_1 a + (\gamma z_R a + \gamma c + x_R b)(\Delta_1 z_R + z_I\Delta_2 + w_R\Delta_3) + (\gamma-1)b(-\Delta_1 Z + z_R(y_R\Delta_3 + x_I\Delta_2))$$

5 Appendix B : Invariance of the determinant of π_*

Let $\mathcal{L}$ be a semisimple Lie algebra with decomposition $\mathcal{L} = \mathcal{K} \oplus \mathcal{P}$ and $[\mathcal{K},\mathcal{K}] \subseteq \mathcal{K}$ and $[\mathcal{K},\mathcal{P}] \subseteq \mathcal{P}$, and consider the conjugacy action of $e^{\mathcal{K}}$ on $e^{\mathcal{L}}$. Consider the natural projection $\pi : e^{\mathcal{L}} \to e^{\mathcal{L}}/e^{\mathcal{K}}$ and $p \in e^{\mathcal{L}}$ a regular point so that at p, π_* is an isomorphism $\pi_* : R_{p*}\mathcal{P} \to T_{\pi(p)}e^{\mathcal{L}}/e^{\mathcal{K}}$. Given bases in $R_{p*}\mathcal{P}$ and $T_{\pi(p)}e^{\mathcal{L}}/e^{\mathcal{K}}$ the matrix $\Pi = \Pi(p)$ representing π_* has determinant which is invariant under the action of $e^{\mathcal{K}}$, i.e., for every $k \in e^{\mathcal{K}}$

$$\det \Pi(p) = \det \Pi(kpk^{-1}).$$

Proof. Let $\{B_1, ..., B_m\}$ be a basis of $\mathcal{P}$ so that $\{R_{p*}B_1, ..., R_{p*}B_m\}$ is a basis of $R_{p*}\mathcal{P}$. Let $x^1, ..., x^m$ be a set of coordinates for $e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$ in a neighborhood of $\pi(p)$. The $m \times m$ matrix Π has entries

$$\Pi_{j,l}(p) = (\pi_* R_{p*} B_l)x^j,$$

and it maps a vector $[\alpha^1, ..., \alpha^m]^T$ representing a tangent vector $V_1 \in R_{p*}\mathcal{P}$, i.e., $V_1 := \sum_{l=1}^m \alpha^l R_{p*}B_l$ to a vector $[r^1, ..., r^m]^T$ representing a tangent vector $V_2 \in T_{\pi(p)}e^{\mathcal{L}}_{reg}/e^{\mathcal{K}}$, i. e., $V_2 = \sum_{j=1}^m r^j \frac{\partial}{\partial x^j}$.

Let $P \in \mathcal{P}$ with $P := \sum_{l=1}^m \alpha^l B_l$. Then, with $k \in e^{\mathcal{K}}$, we obtain [7]:

$$\pi_* R_{p*}P = \pi_* R_{kpk^{-1}} kPk^{-1}.$$

Therefore we have

$$\Pi_{jl}(p) = (\pi_* R_{p*}B_l)x^j = (\pi_* R_{kpk^{-1}*} kB_l k^{-1})x^j =$$
$$(R_{kpk^{-1}*} kB_l k^{-1})x^j \circ \pi = \frac{d}{dt}|_{t=0} x^j \circ \pi(e^{kB_l k^{-1}t} kpk^{-1}).$$

Write kB_lk^{-1} as $kB_lk^{-1} = \sum_{s=1}^m a_l^s B_s$, for an orthogonal matrix a_s^l [8]. Therefore we have

$$\Pi_{jl}(p) = \frac{d}{dt}|_{t=0} x^j \circ \pi(e^{kB_lk^{-1}t} kpk^{-1}) = \frac{d}{dt}|_{t=0} x^j \circ \pi(e^{\sum_{s=1}^m a_l^s B_s t} kpk^{-1}) =$$
$$\sum_{s=1}^m a_l^s \frac{d}{dt}|_{t=0}(x^j \circ \pi(e^{B_s t} kpk^{-1}) = \sum_{s=1}^m a_l^s \Pi_{j,s}(kpk^{-1}).$$

Therefore there exists an orthogonal matrix $A = A(k)$ so that

$$\Pi(p) = \Pi(kpk^{-1})A(k).$$

Taking the determinant of this relation and using $\det(A(k)) = 1$ [9], we obtain $\det(\Pi(p)) = \det(\Pi(kpk^{-1}))$ as desired. □