Control of One and Two Homonuclear Spins

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Abstract

We consider the problem of steering control for the systems of one spin $\frac{1}{2}$ particle and two interacting homonuclear spin $\frac{1}{2}$ particles in an electro-magnetic field. The describing models are bilinear systems whose state varies on the Lie group of special unitary matrices of dimensions two and four, respectively. By performing decompositions of Lie groups, taking into account the describing equations at hand, we derive control laws to steer the state of the system to any desired final configuration. Explicit formulas are given for the parameters involved in the control algorithms. Moreover, the proposed algorithms allow for arbitrary bounds on the magnitude of the controls and for some flexibility in the specification of the final time which must be greater than a given value but otherwise arbitrary.

Keywords: Control of quantum mechanical systems, Particles with spin, Decomposition of Lie groups, Geometric control.

1 Introduction

In recent years, there has been a great amount of interest in the study of control of quantum mechanical systems (see e.g. [1], [3], [23], [33]). This has been motivated by recent advances in the area of nuclear magnetic resonance and laser spectroscopy which have rendered possible the introduction of active control at the atomic level. A major motivation to study control of quantum mechanical system is given by quantum computation [4]. The information in a quantum computer is encoded in the state of a quantum system which has to be manipulated in order to initialize the computer, perform logic operations and measure the result of the computation. Existing techniques for the manipulation of the state of quantum systems only allow to perform very simple operations. On the other hand, the introduction of a control theoretic point of view promises to greatly increase the number of operations that can be implemented with a quantum system as well as their accuracy.
The state of a general multilevel quantum system is described by a vector $|\psi(t)>$, in a finite dimensional Hilbert space. At every time $t$, we have

$$|\psi(t)> = X(t)|\psi(0)>.$$  

(1)

The operator $X(t)$ is the evolution operator solution of the Schrödinger equation

$$i\hbar \dot{X} = HX,$$  

(2)

with initial condition equal to the identity, and $H$ is the Hamiltonian operator. In many experimental situations, such as nuclear magnetic resonance spectroscopy, the Hamiltonian $H$ has the form

$$H := H_0 + \sum_{i=1}^{m} H_i u_i(t)$$

where $u_i(t)$ are externally applied electromagnetic fields which play the role of controls. This simplified model assume no interaction with the environment other than through the controls. In this situation, equation (2) can be written as

$$\dot{X}(t) = AX(t) + \sum_{i=1}^{m} B_i X(t)u_i(t), \quad X(0) = I_{n\times n}.$$  

(3)

In (3), $A, B_1, ..., B_m$, are matrices in $su(n)$, where $n$ is the number of levels of the system under consideration. The solution of (3), $X(t)$, varies on the Lie group of special unitary matrices of dimension $n$, $SU(n)$. In this paper, we are interested in the control of $X$ in (3). This is a way to obtain the control of the state $|\psi>$ in (1) and also to control the operation in (1) to be performed on the state of the quantum system.

Decompositions of Lie groups, and in particular of the Lie group $SU(n)$, have been recently used to prescribe control laws and to study the controllability properties for multilevel quantum systems described by equations such as (3) (see e.g. [14], [15], [24], [25], [29]). To illustrate the basic idea, let us consider the simplest case of a two level quantum system described by

$$\dot{X} = AX + BXu.$$  

(4)

The matrices $A$ and $B$ are in the Lie algebra $su(2)$ and the initial condition is assumed to be the identity. The matrices $A$ and $B$ are linearly independent and therefore they generate the whole Lie algebra $su(2)$, since $su(2)$ has no two dimensional subalgebras.  

Define

$$k := \frac{\sqrt{<A,A>}}{\sqrt{<B,B>}}.$$  

(6)

1If $A$ and $B$ are not linearly independent, the solution of (1), with initial condition equal to the identity, can be written as

$$X(t) = e^{At+B\int_0^t u(\tau)d\tau},$$  

(5)

and, to obtain a desired final configuration, we can just select a control function $u$ to make $At + B\int_0^t u(\tau)d\tau$ equal to one of the logarithms of the desired target $X_f$, if $X_f$ is in the Lie subgroup of $SU(2)$, described by $\{X \in SU(2) | X = e^{Bs}, s \in \mathbb{R}\}$.  

2The inner product $<\cdot, \cdot>$ is defined as $<A,B> := Tr(AB^*)$ and it is equal to the Killing form on $su(2)$ (see e.g. [14]).
The quantity $k$ is a measure of the ‘control authority’ of the given system. The matrices $A + kB$ and $A - kB$ are orthogonal and therefore, if $T_1$ is the unitary matrix which diagonalizes $A + kB$, we have

$$T_1(A + kB)T_1^* = -i\lambda S_z,$$

and

$$T_1(A - kB)T_1^* = -i(aS_y + bS_x),$$

for some parameters $\lambda > 0$, $a, b$ not both zero. $S_x, S_y$ and $S_z$ are the Pauli matrices

$$S_x := \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$S_y := \frac{1}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

$$S_z := \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$  

The matrices $-iS_x$, $-iS_y$, and $-iS_z$ form an orthogonal basis in $su(2)$ and we have the basic commutation relations

$$[-iS_x, -iS_y] := -iS_z, \quad [-iS_y, -iS_z] := -iS_x, \quad [-iS_z, -iS_x] := -iS_y.$$  

Define the unitary matrix

$$T_2 := \begin{pmatrix} 1 & 0 \\ 0 & \frac{a+ib}{\sqrt{a^2+b^2}} \end{pmatrix}.$$  

We have

$$T_2T_1(A + kB)T_1^*T_2^* = -i\lambda S_z,$$  

$$T_2T_1(A - kB)T_1^*T_2^* = -i\sqrt{a^2+b^2}S_y.$$  

In geometric terms, the transformation $T_1$ is a rotation which ensures that the $z$ axis is aligned along the direction specified by $A + kB$ while $T_2$ is a rotation about the $z$ axis to align the direction of rotation specified by $-i(aS_y + bS_x)$ with the $y$ direction. The change of coordinates $T_2T_1$ shows that it is always possible to assume that $A + kB$ and $A - kB$ are proportional to the Pauli matrices $S_z$ and $S_y$, respectively.

Now assume we want to find a control input steering to a final configuration $X_f$ (after the change of coordinates). We can first express $X_f$ using the Euler parametrization of matrices in $SU(2)$ (see e.g. [30])

$$X_f := e^{-iS_x\alpha}e^{-iS_y\beta}e^{-iS_z\gamma},$$

with $\alpha, \gamma \in [0, 4\pi]$, $\beta \in [0, \pi]$. Once the parameters in (16) are known, it is immediate to find a control function steering the state of the system to the value $X_f$. We have the following result.
Theorem 1 The control piecewise constant and equal to $k$ in the interval \( [0, \frac{\gamma}{\lambda}] \), $-k$ in the interval \( \left( \frac{\gamma}{\lambda}, \frac{\gamma}{\lambda} + \frac{\beta}{\sqrt{a^2 + b^2}} \right) \), and equal to $k$ in the interval \( \left( \frac{\gamma}{\lambda} + \frac{\beta}{\sqrt{a^2 + b^2}} + \frac{\alpha}{\lambda} \right) \), steers the state of the system (3) (in the new coordinates) to $X_f$ in (16).

Results similar in spirit to Theorem 1 have appeared in [24] [25]. In particular the paper [25] contains a factorization of the Lie group $SU(2)$ which allows control with arbitrarily bounded power. The authors deal with the case where $A$ and $B$ are orthogonal and then generalize to a large class of system on $SU(2)$.

Consideration of a bounded amplitude control is quite natural in applications like nuclear magnetic resonance where the term $A$ in (4) corresponds to a large constant magnetic field (so that the value of $k$ in (4) is typically large) while the time varying transverse magnetic field $u$ has small amplitude. In the next section, using a Lie group decomposition generalizing Euler decomposition (16) we will give a control algorithm for any system on $SU(2)$ of the form (4) which allows for arbitrary bounds on the control magnitude. Sections 3 through 5 are devoted to the more complicated case of two interacting spin $\frac{1}{2}$ particles. Emphasis is given to the homonuclear case, which for us means that the two particles have the same gyromagnetic ratios. We derive, in Section 3 the model of two interacting spin $\frac{1}{2}$ particles and prove some properties of the Lie algebra $su(n)$ which are relevant for the controllability of this system. The controllability of the system of two homonuclear spin $\frac{1}{2}$ particles is dealt with in detail in Section 4, where we give explicit expressions for the reachable sets at every time. This treatment gives information about what states can be reached at any given time. In Section 5, we present an algorithm to steer exactly the state of this system to any prescribed final condition with arbitrary bounds on the control amplitude. Conclusions are presented in Section 6.

2 Control of two Level quantum Systems with Arbitrarily Bounded Control

Consider once again system (4) that we rewrite here
\[
\dot{X} = AX + BXu,
\] (17)
with $A$ and $B$ in $su(2)$ and linearly independent, and $X(0) = I_{2 \times 2}$. Assume that the amplitude of the control $u$ is bounded by $|u| \leq M$. We will consider a piecewise constant control which attains only the values $\pm M$ (bang-bang). In order to specify the switching times for the bang-bang control, we will consider a decomposition of the Lie group $SU(2)$ in terms of the matrices
\[
Z_1 := A + MB,
\] (18)
\[
Z_2 := A - MB.
\] (19)

In the following we assume that $Z_{1,2}$ are linearly independent matrices in $su(2)$ and we consider the following parameters:
• \(\lambda_{1,2} > 0\) are defined as the magnitudes of the purely imaginary eigenvalues of \(Z_{1,2}\). The one parameter subgroups associated to \(Z_{1,2}\) are periodic with period \(\frac{2\pi}{\lambda_{1,2}}\) and \(\lambda_{1,2}\) is a measure of the speed at which one moves on the one parameter subgroup corresponding to \(Z_1\) and \(Z_2\), respectively.

• The parameter \(\psi\) is the cosine of the angle between \(Z_1\) and \(Z_2\), namely we define

\[
\psi := \frac{<Z_1, Z_2>}{<Z_1, Z_1>^{\frac{1}{2}}<Z_2, Z_2>^{\frac{1}{2}}}. \tag{20}
\]

The parameter \(\psi\) is not changed by a change of coordinates (rotations of the reference frame) nor by a scaling of \(\lambda_1\) and/or \(\lambda_2\). If \(\psi = 0\) then \(Z_1\) and \(Z_2\) are orthogonal. If and only if \(\psi = 1\), \(Z_1\) and \(Z_2\) are proportional to each other which we have excluded so that in general we have \(0 \leq |\psi| < 1\).

Let \(T_1\) be the unitary matrix that diagonalizes \(Z_1\) namely

\[
T_1 Z_1 T_1^* = -i2\lambda_1 S_z, \tag{21}
\]

and define

\[
T_1 Z_2 T_1^* := -i(aS_y + bS_x + cS_z). \tag{22}
\]

With \(T_2\) given by

\[
T_2 := \begin{pmatrix} 1 & 0 \\ 0 & \frac{a+ib}{\sqrt{a^2+b^2}} \end{pmatrix}, \tag{23}
\]

we have

\[
T_2 T_1 Z_1 T_1^* T_2^* = -i2\lambda_1 S_z, \tag{24}
\]

\[
T_2 T_1 Z_2 T_1^* T_2^* = -icS_z - i\sqrt{a^2 + b^2} S_y. \tag{25}
\]

Therefore there exists a unitary matrix \(W := T_2 T_1\) such that

\[
WZ_1 W^* = -i2\lambda_1 S_z, \quad WZ_2 W^* = -icS_z - i\sqrt{a^2 + b^2} S_y := -iD. \tag{26}
\]

The parameters \(\lambda_1, \lambda_2, \psi\) and the matrix \(W\) will all play a role in determining the generalized Euler parameters in the factorization of elements of \(SU(2)\) in terms of \(Z_1\) and \(Z_2\) described in the following theorem.

**Theorem 2.** Consider an arbitrary (target) matrix in \(SU(2)\), \(X_f\) and let \(\alpha \in [0, 4\pi]\), \(\beta \in [0, \pi]\) and \(\gamma \in [0, 4\pi]\) be the Euler parameters of the matrix \(WX_f W^*\), namely

\[
WX_f W^* = e^{-iS_z \alpha} e^{-iS_y \beta} e^{-iS_x \gamma}. \tag{27}
\]

Choose a positive integer \(m\) such that

\[
\cos^2\left(\frac{\beta}{2m}\right) \geq \psi^2. \tag{28}
\]
Then $X_f$ has the following factorization:

$$X_f = e^{Z_1 t_1} (e^{Z_2 t_2} e^{Z_1 t_3})^m e^{Z_1 t_s}, \quad (29)$$

with

$$t_2 := \frac{1}{\lambda_2} \cos^{-1} \sqrt{\frac{1}{1 - \psi^2} \left( \cos^2 \left( \frac{\beta}{2m} \right) - \psi^2 \right)} \quad (30)$$

and setting

$$\phi := \tan^{-1}(-\psi \tan(\lambda_2 t_2)), \quad (31)$$

or

$$\phi := -\text{sign}(\psi) \frac{\pi}{2}, \quad (32)$$

if $\lambda_2 t_2 = \frac{\pi}{2}$,

$$t_1 = t_3 = \frac{\phi}{2\lambda_1}, \quad (33)$$

if $\phi \geq 0$, and

$$t_1 = t_3 = \frac{2\pi + \phi}{2\lambda_1}, \quad (34)$$

if $\phi < 0$.

The proof of the above decomposition is presented in [6]. The described decomposition of the Lie group $SU(2)$ and calculation of the parameters can be easily extended to the Lie group $SO(3)$. The relevant calculations for the latter case are presented in Appendix B.

F. Lowenthal [18] first showed that the Lie group $SU(2)$ is uniformly generated [1] [32] by any two linearly independent matrices in $Z_1 Z_2$. This means that every element $X_f$ of $SU(2)$ can be written as the finite product of alternate elements of the one dimensional subgroups corresponding to $Z_1$ and $Z_2$, namely

$$X_f = e^{Z_1 t_1} e^{Z_2 t_2} e^{Z_1 t_3} \cdots e^{Z_1 t_s}, \quad (35)$$

for some parameters $t_1, t_2, \ldots, t_s > 0$ and that, although $s$ depends on $X_f$, it is uniformly bounded over $SU(2)$. The contribution of Theorem 2 above is that we provide explicit formulas for the parameters $t_j$. The maximum number of factors ‘$s$’ (maximum over all of $SU(2)$) is called order of generation and it is the minimum number of factors needed to express all of the elements of $SU(2)$ as in (35). The order of generation depends on the angle $\psi$ defined as in (20), between $Z_1$ and $Z_2$. In particular, it is minimal and equal to three if $Z_1$ and $Z_2$ are orthogonal. F. Lowenthal in [18] has derived a formula which relates $\psi$ to the order of generation $s$ in (35). In particular, $s = 3$, if $\psi = 0$ and $s = f + 2$ if

$$\cos \left( \frac{\pi}{f} \right) < |\psi| \leq \cos \left( \frac{\pi}{f + 1} \right), \quad (36)$$

with $f \geq 2$. 

6
It is interesting to compare the number of factors for the factorization described in Theorem 2 and the minimum required according to Lowenthal formula (36). The number of factors required in (29) is $2m + 1$ where $m$ is the smallest positive integer satisfying (28). The worst case is when $\beta = \pi$, which shows that the minimum number of factors needed to express all the matrices $X_f$ in $SU(2)$ in the form (29) is $2m + 1$ where $m$ is the smallest integer satisfying

$$|\psi| \leq \cos\left(\frac{\pi}{2m}\right).$$

(37)

A comparison of (37) with (36) shows (identifying $f + 1 = 2m$) that the number of factors needed in our algorithm is exactly the one given by F. Lowenthal, namely the smallest possible, in the case when $f$ in (36) is odd and larger by just one if $f$ is even. In fact, the derivation of Theorem 2 was in the spirit of F. Lowenthal proof of his uniform generation result in [18] [19]. F. Lowenthal uses stereographic projections, translates the problem to the induced subgroup of the Moebius group and uses some of his previous results [17]. Since we are interested in the determination of the parameters involved in the factorization (29), we worked directly on the Lie group $SU(2)$ and derived the factorization using explicit expressions of the matrices involved.

Given the decomposition in Theorem 2, it is now immediate to find a control algorithm to steer the state of system (17). We have the following:

**Theorem 3** Consider the piecewise constant control equal to $M$ for a time $\frac{\alpha_{2\lambda_1}}{2\lambda_1}$, and then equal to $M$, $-M$, $M$ for times $t_3$, $t_2$ and $t_1$, respectively, $m$ times, and then equal to $M$ for an interval of time of length $\frac{\alpha_{2\lambda_1}}{2\lambda_1}$. This control steers the state $X$ of (17) from the identity to $X_f$ in (29).

Notice that Theorem 3 is a direct generalization of Theorem 2 that can be obtained as a special case if $\psi = 0$, $m$ is chosen equal to 1 and one sets $2\lambda_1 = \lambda$, $2\lambda_2 = \sqrt{a^2 + b^2}$. Notice also that, although the algorithm allows to reach a given state $X_f$ at a given time, say $T_f$, one can consider the actual final time as arbitrary as long as it is greater than a given value. This will be very important in the algorithms of Section 5 where we use this flexibility to obtain a given state at a given time in a suitable rotating frame. Let us illustrate this point by assuming (w.l.g.) $Z_1 = -i S_z$, with $S_z$ in (11). Then we have

$$e^{-iS_y\pi} Z_1 e^{iS_y\pi} = -Z_1.$$  

(38)

If we let the system evolve as $e^{Z_1 t}$, for time $\bar{t}$, then steer to $e^{iS_y\pi}$ in time $T_1$, then let the system evolve as $e^{Z_1 t}$ for time $\bar{t}$ and then steer to $e^{-iS_y\pi}$ in time $T_2$, we obtain from (38) the identity matrix in time $2\bar{t} + T_1 + T_2$. If we follow this procedure after having driven the state of the system to $X_f$ in time $T_f$, we steer to $X_f$ in time $T_f + T_1 + T_2 + 2\bar{t}$, with $\bar{t}$ arbitrary. More examples of the use of this procedure will be given in Section 5.

We conclude this section by discussing how the number of factors (switches) needed in the described algorithm, which is, as we discussed above, essentially the minimum number needed, depends on the amplitude of the control. Notice, from formula (28), that
the number of factors $2m+1$ increases with the value of $|\psi|$. By substituting $Z_1 = A+MB$, $Z_2 = A-MB$ in $\psi$ in (11), after some elementary manipulations, we obtain

$$|\psi(M)| := \frac{|k^2 - M^2|}{\sqrt{(k^2 + M^2)^2 - 4M^2(\langle A,B \rangle_{<B,B>})^2}}.$$  

(39)

The parameter $k$ is defined in (6). A study of the function $|\psi|$ in (39) shows that $M = k$ achieves the minimum value of number of switches. The function is decreasing in the interval $[0,k)$ and increasing in $[k, +\infty)$. The number of switches and the number of factors in (35) tends to infinity as $M$ goes to zero as well as $M$ goes to $+\infty$. Therefore, in order to minimize the number of switches, if the control $u$ is bounded by $|u| \leq M$ and $M > k$, it is convenient to use $u = \pm k$ rather than $u = \pm M$. In other terms, there is a natural value for the control, given by $k$ in (6) which is the best to use even though we are allowed higher amplitude controls, as far as the number of switches is concerned.

3 Model of two interacting spin $\frac{1}{2}$ particles

We now turn to the more complicate case of the system of two interacting spin $\frac{1}{2}$ particles used in $NMR$ experiments. Recent literature we will refer to on this topic can be found in [14], [26]. The papers [21], [22] introduce system-theoretic aspects of $NMR$ spectroscopy.

The Hamiltonian of a system of two interacting spin $\frac{1}{2}$ particles which interact with each-other, and are immersed in a driving electro-magnetic field, is given by [2] [8] [10]

$$H(t) := \sum_{k=x,y} (\gamma_1 I_{1k} + \gamma_2 I_{2k}) u_k(t) + (\gamma_1 I_{1z} + \gamma_2 I_{2z}) \bar{u}_z + J I_{1z} I_{2z}.$$  

(40)

The first term on the right hand side of (40) represents the interaction of the two particles with the $x$ and $y$ component of the external magnetic field, $u_x$ and $u_y$, which are allowed to vary with time. The second term represents the interaction with the $z$ component of the field, $\bar{u}_z$, which is kept constant in Nuclear Magnetic Resonance experiments. The last term represents the interaction between the two particles which is modeled with a scalar $Ising$ term. The constants $\gamma_1$ and $\gamma_2$ are the gyromagnetic ratios of particle 1 and 2, respectively. The constant $J \neq 0$ is the coupling constant between the two particles. For $k = x, y, z$, we have

$$I_{1k} := \sigma_k \otimes 1,$$

(41)

and

$$I_{2k} := 1 \otimes \sigma_k,$$

(42)

where $\sigma_k$, $k = x, y, z$, are the components of the spin operator in the $x, y, z$ direction and $1$ is the identity operator. Also, we use the notation

$$I_{1k} I_{2j} := \sigma_k \otimes \sigma_j, \quad j, k = x, y, z.$$  

(43)
Schrödinger equation for the evolution operator \( X \) for this system is given by

\[
\dot{X} = -iH(t)X,
\]

where \( H(t) \) is given in (40). We consider the basis \(|++\rangle, |+-\rangle, |-+\rangle, |--\rangle\) (spin 1 up, spin 2 up and spin 1 up, spin 2 down, and so on), in the underlying four dimensional Hilbert space. In this basis, the matrix representatives of the tensor products in (41), (42), (43) are the Kronecker products of the \( 2 \times 2 \) matrix representatives of the operators that appear as factors, where the matrix representatives of \( \sigma_{x,y,z} \) are given by the Pauli matrices (9) (10) (11). We can write system (40), (44) in the form

\[
\dot{X} = AX + B_x X u_x(t) + B_y X u_y(t) + B_z \bar{u}_z X,
\]

with

\[
A := -iJI_{1z}I_{2z}, \quad B_{x,y,z} = -i(\gamma_1 S_{x,y,z} \otimes 1 + \gamma_2 1 \otimes S_{x,y,z}),
\]

and 1 represents the \( 2 \times 2 \) identity matrix. The state \( X \) of (45) with initial condition equal to the identity, varies on the Lie group \( SU(4) \). It is well known [13] [27] that every state in \( SU(4) \) can be reached from the identity by varying the (arbitrarily bounded) control functions \( u_x(t), u_y(t) \), if and only if the Lie algebra generated by \( \{ A + B_z \bar{u}_z, B_x, B_y \} \), that we will denote here by \( L \), is equal to \( su(4) \). In this case the system is said to be controllable (see also [1], [9], [31] for more explicit controllability criteria for quantum systems). More in general, the set of states that can be obtained with arbitrarily bounded controls for system (45) is the connected subgroup of \( SU(4) \) corresponding to the Lie algebra \( L \). Two cases can be considered: the heteronuclear \( (\gamma_1 \neq \gamma_2) \) and the homonuclear \( (\gamma_1 = \gamma_2) \). We will prove some general properties concerning the Lie algebra structure of these systems and in the next two sections we will study in some detail the controllability properties and give control algorithms for the system of two homonuclear spins.

In order to study the structure of the Lie Algebra underlying system (45), we will need the following general result on the structure of the Lie Algebra \( su(n) \), for general \( n \geq 2 \). The proof is based on the Cartan decomposition [1] of the Lie group \( SU(n) \) and it is presented in [3]. A review of the Cartan decomposition for general semisimple Lie groups can be found in Appendix A.

**Lemma 4** The subalgebra \( so(n) \) and every other element \( f \in su(n), f \notin so(n) \), generate \( su(n) \).

**Proof.** See [3].

For an heteronuclear system \( (\gamma_1 \neq \gamma_2) \), it is easily seen that, with repeated Lie brackets of \( B_x \) and \( B_y \), it is possible to generate all the elements of the form \(-iI_{1k}, -iI_{2k}\) in (10) (12). Therefore, the Lie algebra generated by \( B_x \) and \( B_y \) is given by \( su(2) \times su(2) \). It is known that \( su(2) \times su(2) \) is isomorphic to \( so(4) \), therefore, we would like to use Lemma 4 to conclude that, no matter what the matrix modeling the interaction \( A \notin so(4) \) is, the

\^3We are setting the Planck constant \( \hbar = 1 \).
Lie algebra generated by $A + B_zu_z$, $B_x$ and $B_y$ is equal to $su(4)$. This requires a little care if no further information is provided. Although $su(2) \times su(2)$ is isomorphic to $so(4)$, it might ‘sit’ in $su(4)$ in a different manner from $so(4)$. It turns out that this is not the case since $su(2) \times su(2)$ is in fact conjugate to $so(4)$ via an element of $U(4)$. Therefore we can conclude with the following result which is independent on how we have modeled the interaction in the matrix $A$.

**Theorem 5** For every system of two interacting heteronuclear spins the Lie algebra $L$ is equal to $su(n)$ and the system is controllable.

For homonuclear spins the Lie algebra $L$ associated to the model depends on the type of interaction we consider. For a general interaction of the form $A = -i(aI_1x I_2x + bI_1y I_2y + cI_1z I_2z)$ the Lie algebra $L$ is isomorphic to $u(2)$, if $a = b = c \neq 0$ and to $u(3)$ if at least two of the coefficients $a, b, c$ are different. Let us consider in detail the case of Ising interaction where $a = b = 0$, $c = J \neq 0$.

The matrices $B_{x,y,z}$ are proportional to $-i(S_{x,y,z} \otimes 1 + 1 \otimes S_{x,y,z})$ and $B_x$ and $B_y$ generate a subalgebra isomorphic to $su(2)$ and $so(3)$. For reasons that will be clear shortly, we call this subalgebra $K$. Now write $A := -iJI_1z I_2z$ as

$$ A = A_1 + \frac{1}{3}D, \quad (47) $$

with

$$ A_1 := -\frac{iJ}{3}(2I_{1z}I_{2z} - I_{1x}I_{2x} - I_{1y}I_{2y}), \quad (48) $$

and

$$ D := -iJ \sum_{k=x,y,z} I_{1k}I_{2k}. \quad (49) $$

The matrix $\frac{D}{3}$ commutes with $A_1$ and $B_{x,y,z}$ (and therefore with the Lie algebra generated by them). Repeated Lie brackets of $A_1$ and $B_{x,y,z}$ generate matrices of the form $-i(S_k \otimes S_j + S_j \otimes S_k), j \neq k$, $k \in \{x, y, z\}$ and $-i(S_r \otimes S_r - S_m \otimes S_m), r, m \in \{x, y, z\}$ that span a vector space that we denote by $\mathcal{P}$. Since $A_1 \in \mathcal{P}$, $D \in L$. We define $\mathcal{G} := K \oplus \mathcal{P}$, and we have $[K, K] \subseteq K$, $[K, \mathcal{P}] \subseteq \mathcal{P}$, and $[\mathcal{P}, \mathcal{P}] \subseteq K$. Therefore

$$ L = \text{span}\{\frac{D}{3}\} \oplus \mathcal{G}, \quad (50) $$

and the subalgebra $\mathcal{G}$ has a Cartan decomposition as described in Appendix A.

More information can be obtained on $L$ if we perform a change of coordinates diagonalizing $D$ in $\mathcal{H}$. This transforms the matrix $D$ into $D = -i\frac{2}{3} \text{diag}(-3, 1, 1, 1)$ and all

$^4X \rightarrow TXT^\dagger$ with

$$ T := \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & i & -i & 0 \\ 0 & 1 & 1 & 0 \\ -i & 0 & 0 & -i \\ -1 & 0 & 0 & 1 \end{pmatrix} $$

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the matrices in $\mathcal{G}$ into matrices of the form

$$L := \begin{pmatrix} 0 & 0 \\ 0 & R \end{pmatrix},$$

with $R \in su(3)$. In particular, for matrices in $\mathcal{K}$, $R \in so(3)$, while for matrices in $\mathcal{P}$, $R \in S$, the vector space of $3 \times 3$, zero trace, symmetric, purely imaginary matrices. Therefore, $\mathcal{G}$ is isomorphic to $su(3)$ (notice the fact that all of $su(3)$ is generated can be obtained as an application of Lemma 4) and $\frac{D}{3}$ plays the role of $iI_{3\times3}$. In summary, we have for $\mathcal{L}$ (the symbol $\approx$ indicates Lie algebra isomorphism).

$$\mathcal{L} = \text{span}\{\frac{D}{3}\} \oplus \mathcal{K} \oplus \mathcal{P} \approx u(3) = \text{span}\{iI_{3\times3}\} \oplus su(3) = \text{span}\{iI_{3\times3}\} \oplus so(3) \oplus S. \quad (52)$$

In the following two sections, we focus on controllability analysis and control algorithms for the system of two homonuclear spin $\frac{1}{2}$ particles. A number of algorithms based on Lie group decompositions can be found in the literature for the heteronuclear case (see e.g. [14], [24], [25], [26]). Starting with a decomposition in factors of the target matrix, some algorithms use the so called hard pulses (namely very high amplitude controls) to obtain approximately state transfer within the Lie group corresponding to the Lie algebra generated by the $B$ matrices in a system like (45). This along with zero pulses, which make the state of the system vary on the one dimensional subgroup corresponding to the matrix $A$, can be shown to obtain all the possible targets, if the system is underlying a Cartan decomposition. While this approach has been shown to lead to time optimal controls [14], it has been criticized because of the practical feasibility and possible side effects of the hard pulses. The paper [26] contains a detailed discussion and a comparison between hard pulses and soft pulses control as well as an algorithm for the control of the system of two heteronuclear spin with arbitrarily bounded control. We shall present in Section 5, an algorithm that, without any approximation, steers the system of two homonuclear spin $\frac{1}{2}$ particles to any configuration. This algorithm will be an application of the decomposition of $SU(2)$ described in Theorem 2.

### 4 Controllability analysis

Using the Cartan decomposition for the Lie group $su(3)$ above described, it is possible to obtain more information about the controllability of the system of two homonuclear spins. In particular it is possible to obtain explicit expressions for the reachable sets with piecewise continuous (but not a priori bounded) control. To do so, we will use the main result of [14] which is called there the ‘Time Optimal Tori Theorem’. In the following, we will denote by $\mathcal{R}(t)$ the set of states that can be reached from the identity in time $t$ and by $\mathcal{R}(\leq T)$ the set $\bigcup_{0 \leq t \leq T} \mathcal{R}(t)$. We shall denote by $SU(2)^2$ the Lie group corresponding to the Lie algebra (isomorphic to $su(2)$ and $so(3)$) generated by $\{-i(S_k \otimes 1 + 1 \otimes S_k), k = (x, y, z)\}$, namely the Lie group of matrices of the form $L \otimes L$, with $L \in SU(2)$. This is
a not faithful (2 to 1) representation of \( SU(2) \) and therefore isomorphic to \( SO(3) \). This can also be seen by a change of coordinates as pointed out in the previous section.

**Theorem 7.** For the system of two homonuclear spins, let \( D \) be the matrix defined in (43). For every \( T > 0 \),

\[
\text{clos} \mathcal{R}(T) = e^{\frac{i}{3} DT} \{ X_f \in SU(4) | X_f = K_1 e^{\alpha_1 A_1 + \alpha_2 A_2 + \alpha_3 A_3} K_2 \},
\]

with \( K_{1,2} \in SU(2)^2 \), \( \alpha_{1,2,3} \geq 0 \), \( \alpha_1 + \alpha_2 + \alpha_3 = T \), and

\[
A_1 := A - \frac{1}{3} D = -\frac{iJ}{3} (2I_{1z}I_{2z} - I_{1x}I_{2x} - I_{1y}I_{2y}),
\]

\[
A_2 := -\frac{iJ}{3} (2I_{1y}I_{2y} - I_{1x}I_{2x} - I_{1z}I_{2z}),
\]

\[
A_3 := -\frac{iJ}{3} (2I_{1x}I_{2x} - I_{1z}I_{2z} - I_{1y}I_{2y}).
\]

**Proof.** See [6].

The eigenvalues of the matrices \( A_1 \), \( A_2 \) and \( A_3 \) are given by

\[
\lambda_1 = \lambda_2 = -\frac{1}{6} Ji, \quad \lambda_3 = 0, \quad \lambda_4 = \frac{1}{3} Ji,
\]

therefore the functions \( e^{A_j t} \), \( j = 1, 2, 3 \) are periodic with period \( \frac{12\pi}{|J|} \). This shows that if \( T \geq \frac{36\pi}{|J|} \) in (53) \( \text{clos} \mathcal{R}(T) = e^{\frac{DT}{3}} G \), where \( G \) denotes the Lie group (isomorphic to \( SU(3) \)) corresponding to the Lie algebra \( \mathcal{G} \) isomorphic to \( su(3) \) generated by \( A_1, B_x, B_y \) and \( B_z \). With these notations, we have

**Theorem 8.** If \( T \geq \frac{36\pi}{|J|} \), then

\[
\mathcal{R}(T) = e^{\frac{DT}{3}} G
\]

**Proof.** See [6].

### 5 Control algorithms for two homonuclear spins

In this section we give a constructive control algorithm for the system of two homonuclear interacting spin \( \frac{1}{2} \) particles, which, in the spirit of Theorem 3, allows for arbitrary bounds on the control. This algorithm is based on a Lie group decomposition of the Lie group \( SU(3) \), and on an application of the decomposition result of Theorem 2.

In the following we will set \( \gamma = \gamma_1 = \gamma_2 \). Consider system (43) with \( \gamma_1 = \gamma_2 \) and define

\[
U := e^{\frac{-i}{3} Dt} X.
\]

(59)
Since $D$ commutes with all the matrices in equation (45) we have that $U$ satisfies the equation

$$\dot{U} = A_1 U + B_x U u_x + B_y U u_y + B_z U \bar{u}_z,$$

with $A_1$ given in (54) (see Theorem 7). The matrices $A_1$, $B_x$, $B_y$ and $B_z$ generate a Lie algebra $\mathcal{G}$ isomorphic to $su(3)$ and in particular they are underlying a Cartan decomposition of $\mathcal{G}$, in that $A_1 \in \mathcal{P}$ and $B_x$, $B_y$ and $B_z$ generate $\mathcal{K}$, and $\mathcal{G} = \mathcal{K} \oplus \mathcal{P}$ in the notations of Appendix A. It is also useful to perform a change of coordinates as described in Section 3 diagonalizing the matrix $D$ in (49) as

$$D = -iJ^4 \text{diag}(-3, 1, 1, 1).$$

(61)

This transforms $A$ into the matrix $A = -i \frac{J}{4} \text{diag}(-1, -1, 1, 1)$, and $B_x$, $B_y$ and $B_z$ into the matrices $\gamma S_{2,3}$, $-\gamma S_{2,4}$ and $\gamma S_{3,4}$, respectively, where $S_{j,k}$, $j < k$, denotes the matrix in $so(4)$ with all zero entries except the $(j,k)$-th and the $(k,j)$-th that are equal to 1 and $-1$ respectively. In these coordinates, the matrix defined in (54) is given by $A_1 = -i \frac{J}{4} \text{diag}(0, -\frac{4}{3}, \frac{2}{3}, \frac{2}{3})$. This shows that the Lie group on which the state of the system (60) varies is given by matrices of the form

$$S = \begin{pmatrix} 1 & 0 \\ 0 & G \end{pmatrix},$$

(62)

with $G \in SU(3)$. Therefore we can assume that the target matrix $X_f$ has the form

$$X_f = e^{-\frac{D_T f}{3}} S_f,$$

(63)

where $D$ is now in the new coordinates, $T_f \geq 0$ and $S_f$ has the form in (62). In the system of differential equations in the new coordinates

$$\dot{X} = AX + B_x u_x X + B_y u_y X + B_z \bar{u}_z X,$$

(64)

it will be convenient to scale the time $t$ by a factor $\frac{t}{6}$ and redefine the control functions as $u_x \rightarrow \gamma \frac{6}{\pi} u_x(\frac{6}{\pi} t)$, $u_y \rightarrow -\gamma \frac{6}{\pi} u_y(\frac{6}{\pi} t)$, $\bar{u}_z \rightarrow \gamma \frac{6}{\pi} \bar{u}_z$, which gives simpler expressions for the matrices $A$, $B_{x,y,z}$. In particular, we have that the matrix $B_{x,y,z}$ become

$$B_{x,y,z} = \begin{pmatrix} 0 & 0 \\ 0 & S_{(1,2),(1,3),(2,3)} \end{pmatrix}$$

(65)

where $S_{j,k}$ are the standard basis matrices in $so(3)$. The matrix $D$ becomes $D = -i \frac{J}{4} \text{diag}(-3, 1, 1, 1)$ and the matrix $e^{Dt}$ is periodic with period $\frac{4\pi}{3}$ and therefore $T_f$ in (63) is defined up to multiples of $4\pi$. The matrix $A_1$ takes the simple form $A_1 := A - \frac{D}{3} = \text{id} \text{diag}(0, 2, -1, -1)$. We shall refer to this time scale and control variables in the rest of our treatment.
We now assume that $T_f$ and $S_f$ are given and we show how to steer the state of the system to the desired final configuration (63) with arbitrary bound on the control. We first remark that the problem amounts to the following one:

**Problem 1** Steer the state of the system

\[
\dot{S} = A_1 S + B_x S u_x + B_y S u_y, \tag{66}
\]

from the identity to $e^{-B_z \bar{u}_z (T_f + n4\pi)} S_f$ in time $T_f + 4n\pi$ for sufficiently large $n$, using piecewise constant controls of the form $u_x \equiv 0$, $u_y \equiv $ const, or $u_x \equiv $ const, $u_y \equiv 0$.

To see this, define

\[
S := e^{(-\frac{1}{2}D - B_z \bar{u}_z) t} X, \tag{67}
\]

and using (64), $S$ satisfies

\[
\dot{S} = A_1 S + e^{-B_z \bar{u}_z t} B_y e^{B_z \bar{u}_z t} S u_y(t) + e^{-B_z \bar{u}_z t} B_x e^{B_z \bar{u}_z t} S u_x(t). \tag{68}
\]

In deriving (68) we have used the fact that $B_z$ commutes with $A$ and $D$ commutes which each one of the matrices in equation (64). Now a direct calculation shows that if $u_x(t) = \tilde{k}\cos(\bar{u}_z t)$ and $u_y = -\tilde{k}\sin(\bar{u}_z t)$ then the last two elements in the above equation give $\tilde{k} B_x S$, and if $u_x(t) = \tilde{k}\cos(\bar{u}_z t)$ and $u_y(t) = \tilde{k}\sin(\bar{u}_z t)$ the last two terms give $\tilde{k} B_y S$. Therefore, if one keeps switching between these two types of controls the right hand side of equation (68) is alternatively of the form $A_1 S + \tilde{k} B_x S$ and $A_1 S + \tilde{k} B_y S$, where we have denoted by $\tilde{k}$ any constant. Therefore the choice of the control reduces to the choices of the constants $\tilde{k}$. These calculations could have been carried out in the original coordinates and are often referred to in the physics literature as ‘considering the system in a rotating frame’ [26]. We emphasize that the calculations in the case considered here do not involve any approximation.

Now, if we are able to steer the state of the system (66) or equivalently the state of (38) with the above described controls to $e^{-B_z \bar{u}_z (T_f + 4n\pi)} S_f$ in time $T_f + 4n\pi$, it follows from (67) that the state of the original system (64) is driven to $e^{\frac{1}{2}DT_f + 4n\pi D} S_f = e^{\frac{1}{2}DT_f} S_f$, because of the periodicity of $e^{DT}$.

**Solution to Problem 1**

Notice that, in the new coordinates, the first rows and columns of the matrices $A_1$, $B_x$ and $B_y$ are zeros, so that we can consider the system as a $3 \times 3$ one with state varying on $SU(3)$.

We show next, how to obtain every matrix of the form $e^{B_z t} = e^{S_{1,2} t}$ (notations are for $3 \times 3$ matrices). Set $u_y \equiv 0$ and write $A_1 = -F + \tilde{A}_1$, with $F = -idiag(\frac{1}{2}, \frac{1}{2}, -1)$ and $\tilde{A}_1 = -idiag(\frac{-3}{2}, \frac{3}{2}, 0)$. Setting

\[
\tilde{S} := e^{F t} S \tag{69}
\]

and noticing that $F$ commutes with both $A_1$ and $B_x$, we obtain

\[
\tilde{S} = \tilde{A}_1 \tilde{S} + B_x \tilde{S} u_x. \tag{70}
\]
Now, since the third rows and columns of system (70) are all zeros the system is essentially 2 × 2 and the matrices are essentially in \( su(2) \). Therefore, we can apply Theorems 2 and 3 to steer the state of this system from the identity to the matrix
\[
e^{B_x t} := \begin{pmatrix}
\cos(t) & \sin(t) & 0 \\
-\sin(t) & \cos(t) & 0 \\
0 & 0 & 1
\end{pmatrix}.
\]

(71)

Let \( T_x = T_x(t) \), the time needed to steer to \( e^{B_x t} \) with bound on the control, according to Theorems 2 and 3. Now, notice that \( e^{-B_x \frac{\pi}{2}} \tilde{A}_1 e^{B_x \frac{\pi}{2}} = -\tilde{A}_1 \) and therefore, for every \( \tau \geq 0 \), we have
\[
e^{\tilde{A}_1 \tau} e^{-B_x \frac{\pi}{2}} e^{\tilde{A}_1 \tau} e^{B_x \frac{\pi}{2}} = I_{3 \times 3}.
\]

(72)

Therefore, we can steer to the identity in time
\[
T_{Id}(\tau) := 2\tau + T_x\left(\frac{\pi}{2}\right) + T_x\left(\frac{3\pi}{2}\right)
\]

(73)

with \( \tau \geq 0 \) arbitrary. We would like to steer the state of (70) to \( e^{B_x t} \) in time \( 4\bar{n}\pi \), for some integer \( \bar{n} \). We can do that by steering in time \( T_x(t) \) to \( e^{B_x t} \) and then by steering (from the identity) to the identity in time \( T_{Id}(\tau) \) in (73), choosing \( \tau \) so that
\[
T_x(t) + T_{Id}(\tau) = 4\bar{n}\pi.
\]

(74)

Notice that, from the decomposition of Theorem 2, the time \( T_x(t) \) is uniformly bounded (as \( 0 \leq t \leq 2\pi \)) by a value \( \bar{T}_x \) that depends on the bound on the control. \( \bar{T}_x \) can be easily calculated by knowing the order of generation in terms of the two generating one-dimensional subgroups and knowing their periods. Therefore, we can always assume that \( \bar{n} \) is chosen so that we can make (74) satisfied for every \( t, 0 \leq t \leq 2\pi \), for appropriate \( \tau \), namely \( 4\bar{n}\pi \geq \bar{T}_x + T_x\left(\frac{\pi}{2}\right) + T_x\left(\frac{3\pi}{2}\right) \). We will assume this to be the case in the following.

Now, since \( e^{Ft} \) is periodic with period \( 4\pi \), by steering the state \( \tilde{S} \) of (70) to \( e^{B_x t} \) in time \( 4\bar{n}\pi \), using (69), we have steered the state of the system (66) to \( e^{B_x t} \) in time \( 4\bar{n}\pi \).

In a completely analogous way, one can obtain matrices of the form \( e^{B_y t} = e^{S_{1,3}t} \) in time \( 4\bar{n}\pi \) (in fact the procedure is completely equivalent and the value of \( \bar{n} \) is the same in the two cases). Moreover, noticing that
\[
e^{B_x \frac{\pi}{2}} e^{B_y t} e^{-B_x \frac{\pi}{2}} = e^{B_z t} := e^{S_{2,3}t},
\]

(75)

one can obtain every matrix of the form \( e^{B_z t} \) in time \( 3 \times 4\bar{n}\pi \).

At this point, we recall a decomposition of the matrices \( U_f \in SU(3) \) presented in (65). Every matrix \( U_f \in SU(3) \) can be written as
\[
U_f = D(\alpha_1, \alpha_2, \alpha_3)U_{12}(\theta_1, \sigma_1)U_{13}(\theta_2, \sigma_2)U_{23}(\theta_3, \sigma_3),
\]

(76)

An alternative here could have been to apply the algorithm of [24] appropriately modified to allow bounds on magnitude rather than power. This is possible since in this case the two matrices \( A_1 \) and \( B_x \) are orthogonal.
where the matrices $U_{kl} (\theta, \sigma)$, with $k < l$ are the matrices whose submatrix intersection of the $k$–th and $l$–th rows and columns is given by

$$L := \begin{pmatrix} \cos(\theta) & -\sin(\theta) e^{-i\sigma} \\ \sin(\theta) e^{i\sigma} & \cos(\theta) \end{pmatrix},$$

(77)

so that, for example

$$U_{12}(\theta_1, \sigma_1) := \begin{pmatrix} \cos(\theta_1) & -\sin(\theta_1) e^{-i\sigma_1} \\ \sin(\theta_1) e^{i\sigma_1} & \cos(\theta_1) \end{pmatrix} \quad (78)$$

The matrix $D(\alpha_1, \alpha_2, \alpha_3)$ is of the form

$$D(\alpha_1, \alpha_2, \alpha_3) := \begin{pmatrix} e^{i\alpha_1} & 0 & 0 \\ 0 & e^{i\alpha_2} & 0 \\ 0 & 0 & e^{i\alpha_3} \end{pmatrix},$$

(79)

with $\alpha_1 + \alpha_2 + \alpha_3 = 0$. Once $U_f$ is given, the parameters $\theta_j, \sigma_j, \alpha_j$, $j = 1, 2, 3$, can be easily calculated by an analytic procedure described in [20]. Therefore, specifying $U_f$ is equivalent to specifying the parameters $\theta_j, \alpha_j, \sigma_j$.

Now notice that

$$U_{12}(\theta_1, \sigma_1) = e^{A_1 \frac{\theta_1}{3}} e^{B_\sigma \theta_1} e^{A_1 t}.$$

(80)

Therefore the matrix $U_{12}(\theta_1, \sigma_1)$ can be obtained (assume w.l.g. $\sigma_1 \geq 0$) by letting the system go with $u_x \equiv u_y \equiv 0$, for time $\frac{\theta_1}{3}$, and then drive the system to $e^{B_\sigma \theta_1}$ as explained above, and then let the system go again for time $2\pi - \frac{\theta_1}{3}$, setting $u_x \equiv u_y \equiv 0$ again. The same thing can be done for the terms $U_{13}(\theta_2, \sigma_2)$ and $U_{23}(\theta_3, \sigma_3)$, in (76), with $e^{B_\sigma \theta_2}$ and $e^{B_\sigma \theta_3}$ replacing $e^{B_\sigma \theta_1}$, respectively. Therefore the last three factors in (76) can be written as

$$D(-\alpha_1, -\alpha_2, -\alpha_3) U_f = e^{A_{1t_1}} e^{B_{\sigma t_2}} e^{A_{1t_3}} e^{B_{\sigma t_4}} e^{A_{1t_5}} e^{B_{\sigma t_6}} e^{A_{1t_7}}.$$

(81)

Our previous discussion shows how to calculate the parameters $t_j \geq 0$, $j = 1, ..., 7$ and how to drive the identity to each one of the factors in (81). Recalling periodicity of the matrix $e^{A_x t}$ and the times to drive to the matrices $e^{B_{\sigma t_2}}$, $e^{B_{\sigma t_4}}$, $e^{B_{\sigma t_6}}$, calculated in the above discussion, the transfer to a matrix of the form (81) takes at most time

$$\bar{T}_1 = 4 \times 2\pi + 2 \times 4\tilde{n}\pi + 3 \times 4\tilde{n}\pi,$$

(82)

where the three terms on the right hand side refer to the matrices of the form $e^{A_x}$, $e^{B_{\sigma t}}$ and $e^{B_{\sigma t}}$, and $e^{B_{\sigma t}}$, respectively. Now, the matrix $D(\alpha_1, \alpha_2, \alpha_3)$, with $\alpha_1 + \alpha_2 + \alpha_3 = 0$, can be obtained as

$$D(\alpha_1, \alpha_2, \alpha_3) = e^{B_{\sigma} \frac{\theta_1}{3}} e^{A_{1t_1}} e^{-B_{\sigma} \frac{\theta_1}{3}} e^{A_{1t_2}},$$

(83)

if $2t_2 - t_1 = \alpha_1$ and $2t_1 - t_2 = \alpha_2$. Therefore the overall transfer of the state of (66) from the identity to $U_f$ takes at most time

$$\bar{T} = \bar{T}_1 + 2 \times 4\tilde{n}\pi + 2 \times 2\pi,$$

(84)
with $T_1$ defined in (82).

Now notice that, for every $\tau \geq 0$, we have

$$e^{B_1 \tau} e^{A_1 \tau} e^{-B_2 \tau} e^{-B_1 \tau} e^{B_2 \tau} e^{A_1 \tau} = I_{3 \times 3}.$$ \hfill (85)

Therefore the Identity matrix can be obtained in time $3\tau + 4 \times 4\tilde{n}\pi$, for arbitrary $\tau \geq 0$.

Now choose $n$ so that

$$T_f + 4n\pi \geq \tilde{T} + 4 \times 4\tilde{n}\pi,$$ \hfill (86)

and express the matrix $e^{-B_z \tilde{n}_z(T_f + 4n\pi)} S_f$ as $U_f$ in (76). Then, we have showed how in time at most $\tilde{T}$ we can steer to this final condition. Let $\hat{T}$ ($\leq \tilde{T}$) the time actually used to steer to $e^{-B_z \tilde{n}_z(T_f + 4n\pi)} S_f$, and let us define

$$\tilde{t} := T_f + 4n\pi - \hat{T} - 4 \times 4\tilde{n}\pi \geq 0,$$ \hfill (87)

from (86). Then by steering to the identity in time $\tilde{t} + 4 \times 4\tilde{n}\pi$, we have driven the state of the system (66) to $e^{-B_z \tilde{n}_z(T_f + 4n\pi)} S_f$, in time exactly $T_f + 4n\pi$, as desired. $\square$

6 Conclusions

We have presented control algorithms and controllability analysis for the systems of one and two homonuclear spin $\frac{1}{2}$ particles in a magnetic fields. In particular explicit expressions for the reachable sets have been obtained.

The control algorithms are based on a Lie group decomposition of the Lie group $SU(2)$ for which we have obtained explicit expressions of the parameters involved. All the algorithms described allow for arbitrary bounds on the controls and provide explicit expressions for the parameters involved in the control design. Moreover, the algorithms allow some flexibility in the final time that can be fixed a priori as long as it is greater than a given value. This is due to the right invariance of the systems considered and to the fact that the identity matrix can be obtained in sufficiently large but otherwise arbitrary time. Questions of optimization of the time transfer have not been considered here and will be object of future research. Also, the explicit generation of control protocols which use the decompositions of $SU(2)$ described here as a basic building block for different and more complicated systems will be investigated.

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Appendix A: Review of Cartan decomposition of Lie groups

We review, in this Appendix some basic facts about decompositions of Lie groups based on symmetric spaces, also known as Cartan decomposition, that we will use in the following. We refer to the texts [11] [12] for further details and generalizations as well as for some of the terminology that we use here. Applications to control theory are considered in [4] [32].

Consider a semisimple Lie algebra $\mathcal{G}$ and the corresponding connected Lie group $G$. Assume that $G$ admits a decomposition as a vector space

$$\mathcal{G} = \mathcal{K} \oplus \mathcal{P},$$

(88)

where $\mathcal{K}$ is subalgebra of $\mathcal{G}$, namely $[\mathcal{K}, \mathcal{K}] \subseteq \mathcal{K}$. Moreover, assume that the following commutation relations hold among the elements of $\mathcal{K}$ and $\mathcal{P}$,

$$[\mathcal{K}, \mathcal{P}] \subseteq \mathcal{P},$$

(89)

$$[\mathcal{P}, \mathcal{P}] \subseteq \mathcal{K}.$$  

(90)

Denote by $K$ the connected Lie group corresponding to $\mathcal{K}$ and assume it is compact. Denote by $P$ the image of $\mathcal{P}$ under the exponential map. Under the above assumptions and definitions,

$$G = PK,$$

(91)

namely every element of $G$ can be written as the product of an element of $P$ and an element of $K$.

Every element in $P$ belongs to a Cartan subalgebra (namely a maximal Abelian subalgebra) $\mathcal{A}$ whose dimension is called the rank of the Lie group $G$. Moreover, any two Cartan subalgebras are conjugate via elements in $K$, namely, if $\mathcal{A}'$ is another Cartan subalgebra, then there exists an element $K \in K$ such that $KAK^{-1} \in \mathcal{A}'$, for each $A \in \mathcal{A}$. As a consequence, every element $P$ in $P$, can be written as $P = KAK^{-1}$, where $K$ is an element of $K$ and $A$ is an element of $\mathcal{A}$, the connected Lie subgroup of $G$ associated to $\mathcal{A}$. Therefore, one can write

$$G = KAK,$$

(92)

namely, every element in $G$ can be written as the product of an element in $K$, an element in $A$ and an element in $K$, in that order.

The simplest example of Cartan decomposition (92) is Euler decomposition for $SU(2)$. Consider the Pauli matrices in (9), (10), (11), divided by $i$, $-iS_x$, $-iS_y$, $-iS_z$. These matrices satisfy the commutation relations (12). Therefore, one can take, for example, $\mathcal{K} := span\{S_y\}$, and $\mathcal{P} := span\{S_x, S_z\}$, and $\mathcal{A} := S_z$, although every other combination would be possible.

The decomposition (92) can be continued by decomposing $K$ in the same fashion as $G$. Continuing this way, one end up with an expression of every element of the Lie group $G$ in terms of the product of elements belonging to one dimensional subgroups.
Appendix B: A decomposition of $SO(3)$

In the following we shall call $S_{hk}, h < k$ the matrix $\in so(3)$ which has zeros everywhere except in the $h,k$-th ($k,h$-th) entry which is equal to 1 ($-1$). Given a matrix $Z_1$, there exists a matrix $T_1 \in SO(3)$ such that

$$T_1 Z_1 T_1^T := \lambda_1 S_{12},$$

(93)

$\lambda_1 > 0$. This can be easily seen by choosing $T_1 := [v_1, v_2, v_3]^T$, with $v_3$ such that $v_3^T Z_1 = 0$ and with norm equal to one and $v_1$ and $v_2$ such that $\{v_1, v_2, v_3\}$ form an orthonormal basis in $\mathbb{R}^3$. We also set

$$T_1 Z_2 T_1^T := a S_{12} + b S_{13} + c S_{23},$$

(94)

Choose now $T_2 := e^{S_{12} \theta}$ with $\theta$ such that $bc \cos(\theta) + cs \sin(\theta) = 0$. Then we have

$$T_2 T_1 Z_1 T_1^T T_2^T := \lambda_1 S_{12},$$

(95)

$$T_2 T_1 Z_2 T_1^T T_2^T := a S_{12} + d S_{23},$$

(96)

for some parameter $d \neq 0$. Therefore, we can always assume that, in appropriate coordinates, the matrices $Z_1$ and $Z_2$ have the form $Z_1 := \lambda_1 S_{12}$ and $Z_2 := a S_{12} + d S_{23}$, respectively. Moreover we can divide $Z_1$ by $\lambda_1 > 0$ (this has the only effect that, in the matrices if the form $e^{Z_1 t}$, $t$ has to be scaled by a factor $\lambda_1$) and analogously we can divide $Z_2$ (in the new coordinates in (96)) by $d$ and therefore the parameter $t$ in the subgroup $e^{Z_2 t}$ has to be scaled by a factor $d$. Define $\rho := \frac{a}{d}$, we can assume, without loss of generality, that the matrices $Z_1$ and $Z_2$ are given by $Z_1 := S_{12}$ and $Z_2 := \rho S_{12} + S_{23}$, and we shall do so in the following. Notice also that the above manipulations do not modify the value of the parameter $\psi$ in (20) which is given, in terms of $\rho$, by

$$\psi := \frac{\rho}{\sqrt{1 + \rho^2}}.$$  

(97)

To express a matrix $X_f \in SO(3)$ as

$$X_f = e^{Z_{1 t_1}} e^{Z_{2 t_2}} e^{Z_{1 t_3}} \cdots e^{Z_{1 t_s}},$$

(98)

we first recall (see e.g. [30]) that we can express every matrix $X_f \in SO(3)$ as

$$X_f = e^{S_{12} \alpha} e^{S_{23} \beta} e^{S_{12} \gamma},$$

(99)

with $\alpha, \gamma \in [0, 2\pi]$ and $\beta \in [0, \pi]$. This is the classical Euler decomposition of a rotation. The Euler parameters $\alpha, \beta$ and $\gamma$ can be easily calculated by using an analytic procedure described in [28]. Now, since we have set $Z_1 = S_{12}$, the problem is to express every matrix of the form $X_f = e^{S_{23} \beta}$ as in (98). To do that, we show how to express every matrix of the form $e^{S_{23} \frac{\beta}{m}}$ as

$$e^{S_{23} \frac{\beta}{m}} = e^{Z_{1 t_1}} e^{Z_{2 t_2}} e^{Z_{1 t_3}},$$

(100)
for sufficiently large \( m \). An explicit calculation gives

\[
e^{Z_{2t_2}} = \begin{pmatrix}
\frac{1+\rho^2 c}{\eta^2} & \frac{\rho s}{\eta} & \frac{\rho - \rho c}{\eta^2} \\
\frac{-\rho s}{\eta} & c & \frac{2}{\eta} \\
\frac{-c \rho + \rho}{\eta^2} & \frac{-s}{\eta} & \frac{c + \rho^2}{\eta^2}
\end{pmatrix},
\]

(101)

where \( \eta := \sqrt{1 + \rho^2} \), \( s := \sin(\eta t_2) \), \( c := \cos(\eta t_2) \). Now, if we choose \( m \) so that

\[
2\psi^2 - 1 \leq \cos\left(\beta \frac{\eta}{m}\right),
\]

(102)

we can choose \( t_2 \) so that

\[
\frac{c + \rho^2}{\eta^2} := \frac{\cos(\sqrt{1 + \rho^2 t_2}) + \rho^2}{1 + \rho^2} = \cos\left(\beta \frac{\eta}{m}\right).
\]

(103)

Assume that this is the case and consider \( e^{Z_{2t_2}} \) in (101) with this choice. For brevity, let us call \( a_{ij} \) its \( i,j \)-th element. By choosing \( t_1 \) so that \( \cos(t_1)a_{13} + \sin(t_1)a_{23} = 0 \), we can make the 1,3-th entry of the matrix \( e^{Z_{t_1}}e^{Z_{2t_2}} \) equal to zero. The 2,3-th entry of this matrix is equal to \( \sin(t_1)a_{13} + \cos(t_1)a_{23} \) and it is equal to \( \sin(\beta \eta/m) \) up to the sign that can be changed by replacing \( t_1 \) with \( t_1 + \pi \). Let us now denote by \( a_{ij} \) again the entries of the new matrix \( e^{Z_{t_1}}e^{Z_{2t_2}} \). By choosing \( t_3 \) so that \( a_{11}\sin(t_3) + a_{12}\cos(t_3) = 0 \), we can make the 1,2-th entry of the matrix \( e^{Z_{t_1}}e^{Z_{2t_2}}e^{Z_{t_3}} \) equal to zero, without affecting the 1,3-th, 2,3-th and 3,3-th entries (this procedure is reminiscent of the standard calculation of Euler angles in [28]). The resulting matrix is exactly \( e^{S_{2\beta}} \). Therefore, by considering \( m \) factors, a constructive decomposition of \( SO(3) \) has been obtained.