Control of a Coupled Two Spin System Without Hard Pulses

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Abstract

Constructive techniques for controlling a coupled, heteronuclear spin system, via bounded amplitude sinusoidal pulses are presented. The technique prepares exactly any desired unitary generator in a rotating frame, through constant controls. Passage to the original coordinates provides a procedure to prepare arbitrary unitary generators, via bounded amplitude piecewise sinusoidal pulses whose frequency is one of the two Larmor frequencies and whose phase takes one of two values. The techniques are based on a certain Cartan decomposition of $SU(4)$ available in the literature. A method for determining the parameters entering this Cartan decomposition, in terms of the entries of the target unitary generator, is also provided.
1 Introduction

The goal of this paper is to provide, constructively and exactly (i.e., without any approximations) a decomposition:

\[ e^{-iL_{ij}} = \Pi_{k=1}^{Q} e^{-ia_kI_1zI_2z - ib_kI_{ij}}, i = 1, 2; j = x, y \]  

(1.1)

satisfying i) O1 \( a_k > 0 \); and ii) O2 \( |b_k| \leq C \), for some prescribed bound \( C \). The matrices, \( I_{ij}, i = 1, 2; j = x, y, z \), defined in Section 2, are the standard tensor products of \( I_2 \) and the Pauli matrices. As will become clear, later the same decomposition can be refined to simultaneously satisfy \( \left| \frac{b_k}{a_k} \right| \leq D \) for another bound \( D \). This problem arises in the control of a coupled, heteronuclear, two spin system which is being controlled by addressing each spin individually. The adjective “heteronuclear” is, throughout this paper, meant only to signify that the Larmor frequencies of the two spins are different. The condition O1 just means that the time for which a pulse has to be applied must necessarily positive, while O2 (or more precisely, the condition \( \left| \frac{b_k}{a_k} \right| \leq D \)) represents the fact that hard pulses are not being used.

Coupled spin systems are useful from several points of view. They are certainly ubiquitous in NMR studies. [1, 2]. They also provide examples of coupled qubits in quantum computation and information processing. [3, 4, 5, 6]. One method to control spin systems is to use hard pulses, i.e., high amplitude pulses applied for very short times. The usage of hard pulses, though useful from the perspective of minimizing the time consumed to prepare a desired unitary generator, \( S \), has its own problems. Perhaps most importantly, the usage of hard pulses allows one to only approximately prepare \( S \), since the available resources in any situation is limited. For certain problems of NMR spectroscopy this may not be such a big restriction since the translation of a certain NMR objective to the problem of unitary generator preparation may allow for a broad choice of unitary generators (though, to the best of our knowledge, there has been no systematic assessment of the inaccuracies introduced by the usage of hard pulses for specific NMR objectives). However, for purported quantum computation applications it is indeed a restriction, since the desired \( S \) has to be obtained with great accuracy. Secondly, the usage of hard pulses may
violate the basic feature assumed often in the methodology - namely the ability to address single spins selectively. This already necessitates restriction to heteronuclear molecules. However, even for heteronuclear molecules the usage of infinite amplitude is problematic. Indeed, neglecting modes which are coupled to a system being studied is essentially a perturbation theory argument. Thus, not only has the frequency of the pulse got to be in resonance with the subsystem being studied, but the pulse area has also got to be bounded. If high amplitudes are being used then the pulse has to be applied for an extremely short time. It is unrealisitic to assume that a pulse can be applied for an infinitesimal time in the laboratory. The situation is analogous to the usage of the rotating wave approximation in molecular control studies, \[7, 8, 9\]. Not only must there be no resonances amongst the coupled levels, but the amplitude of the pulse must be much smaller than the frequency separation between the pair of levels being addressed. Similar considerations occur in NMR spectroscopy, \[10\]. These problems are compounded further in quantum computation applications, since it is desirable to perform local operations on individual (or small collections of) qubits, without too much crosstalk with other qubits during these operations. Usage of hard pulses, will eventually cause other qubits to be coupled. Put differently, one of the goals of hard pulse technology, namely the avoidance of decoherence effects, can in fact be defeated by the very usage of hard pulses. Thus, while it is desirable to finish all control action before relaxation processes become dominant, it is even more important to use fields which do not cause other couplings or processes neglected in a model to become significant. Quite often this means essentially that the field be bounded in amplitude. In this paper, arbitrary bounds on the amplitude will be allowed. Thus, while \(\omega_1 \neq \omega_2\) (where the \(\omega_i\), \(i = 1, 2\) are the individual frequencies) is needed, the difference need not be as large, as would be required by the usage of hard pulses. Thus, there is lots to be said for controlling spin systems without hard pulses. In this paper, explicit techniques which avoid hard pulses are provided for a coupled spin system.

It is worthwhile to place in proper mathematical context the question being studied. Coupled two spin systems can be viewed as examples of left-invariant systems, with drift, evolving on the compact Lie group, \(SU(4)\), \[13\]. It is known non-constructively that,
under a certain Lie algebraic condition, such systems can be controlled with piecewise constant pulses whose amplitude can be arbitrarily bounded \[11\]. Providing constructive proofs for such results, on the other hand, is an entirely different matter. There are two sources of complication. First, the ambient Lie group, \(SU(4)\), is high-dimensional (precisely, fifteen dimensional). But more importantly, the presence of a drift term (i.e., the free Hamiltonian) significantly complicates constructive control. Indeed, from a control theoretic perspective hard pulse arguments are ways of avoiding the effects of drift (though at the expense of introducing far more deleterious effects). There is an extensive literature on constructive control for driftless systems - see, for instance, the survey, \[12\]. The same reference contains a survey of special classes of classical mechanical systems with drift, which can be controlled constructively. In \[13\], building on earlier work \[8\], a detailed study of constructive control of systems with drift on \(SU(2)\) was provided. The special structure of \(SU(2)\) played a crucial role in this effort. In this paper, we will show that the special structure of \(SU(2)\) allows, once again, to constructively control the spin system being studied here. This structure of \(SU(2)\) enters in two manners. First, the groups \(SU(4)\) and \(SO(4)\) are intimately connected to one another due to one well-known Cartan decomposition of \(SU(4)\). This Cartan decomposition factors every \(S \in SU(4)\) as products of matrices in \(SO(4)\) and matrices which are exponentials of a Cartan subalgebra of the complement of \(so(4)\), the Lie algebra of \(SO(4)\), in \(su(4)\), the Lie algebra of \(SU(4)\) \[14, 15, 16\]. Now \(SO(4)\) is essentially the same as \(SU(2) \otimes SU(2)\). Not only does this fact clearly establish this Cartan decomposition (this is well known), but it also enables techniques inspired by our earlier paper, \[13\], for systems on \(SU(2)\) to achieve the main goals of this paper. The second role of \(SU(2)\) is to facilitate the calculation of the real parameters in this Cartan decomposition. In the appendix, a method to determine these parameters as explicitly as possible (explicit modulo the solution of a pair of transcendental equations) is provided, and once again the structure of \(SU(2)\) is the main ingredient.

In \[17\] the authors use this particular Cartan decomposition of \(SU(4)\) to address the problem of generating any unitary generator \(S \in SU(4)\) for a coupled two particle spin system via selective one-spin hard pulses. The essential difference between the approach
taken here and that in [17] stems from a Lie theoretic nuance and may be summarized as follows. This Cartan decomposition and plus a few calculations leads to a factorization of any \( S \in SU(4) \), [17]:

\[
S = \prod_{k=1}^{Q} \exp(-it_kA_k)
\]

(1.2)

where each \( A_k \) is one of \( I_{1z}I_{2z}, I_{1x}, I_{2x}, I_{1y}, I_{2y} \). Greater detail about the decomposition, (1.2), is provided in Equation (2.10) in the next section. Under the assumption that it is possible to address single spins selectively, (and a subsequent passage to a rotating frame) \( I_{1z}I_{2z} \) represents the internal Hamiltonian, whereas the remaining matrices represent the control coupling. In [17] factors of the type \( \exp(-it_kI_{1z}I_{2z}) \) are generated by free evolution, whereas factors which are exponentials of the control couplings are generated by hard pulses, so that the drift term, i.e., \( I_{1z}I_{2z} \), makes a negligible contribution to such a factor. This, naturally, makes the generation of the desired \( S \) (even in the rotating frame) at best approximate. In our approach, we will also generate the factors \( \exp(-it_kI_{1z}I_{2z}) \) through free evolution. However, instead of viewing the remaining factors as the exponentials of the control couplings, we view them as the exponentials of the iterated commutator of the internal Hamiltonian and the control couplings. In this iterated commutator, the internal Hamiltonian occurs twice whereas the control couplings occur only once. Thus it may be surmised, based on our prior experience [13], that such exponentials can be generated via three factors, two of which are free evolution terms and one is a control (though not hard) pulse. While, this conjecture has not been established for general nonlinear control systems, it turns out to be valid for the two spin system studied in this paper. Put differently, in generating the exponentials of the control couplings we make systematic use of the drift term, as opposed to treating it as a nuisance which can be overcome via hard pulses. As a further step towards making the whole procedure constructive methods which yield the \( t_k \) in Equation (1.2) in terms of the entries of the target unitary generator, \( S \), will be displayed. The fact that the Cartan decomposition is the analogue of the Euler decomposition for the higher dimensional unitary groups is well known, [14, 15, 16]. However, a stumbling block in its usage is the fact that the analogues of the Euler angles, i.e., the real parameters \( t_k \), have never been explicitly written down in terms of the entries
of the target matrix $S$.

Ultimately, the choice of hard versus soft pulses depends on both the system and the target in question. The contribution of this paper is to show that many objectives can be met via soft pulses. Furthermore, this is demonstrated by making use of the iterated commutators of the internal Hamiltonian and the control Hamiltonians, in contrast to hard pulse approaches which make no use of this commutator. This is another reason why the results below may be of interest. Indeed, all arguments for the controllability of finite dimensional quantum systems [11, 18, 19, 20, 21, 22] hinge on the commutators of the internal Hamiltonian with the control Hamiltonians. Further, these arguments also show that it is possible (non-constructively) to prepare any target via bounded amplitude fields. Thus, it is at least didactically pleasing to demonstrate controllability constructively via methods which explicitly use such iterated commutators. In summary, two important problems are solved constructively in this paper: a) the control of a coupled spin system via sinusoidal, bounded amplitude pulses assuming the factors $t_k$ of Equation (1.2) are given, and b) finding these parameters, $t_k$, algorithmically (so that there is something useful even for aficionados of hard pulses). For both these problems a significant role is played by the structure of $SU(2)$.

The balance of this paper is organized as follows. In the next section some notation and basic facts about the Lie group $SU(2)$ will be collected. In particular, an explicit formula for an Euler angle factorization, with factors exponentials of $\sigma_x$ and $\sigma_y$, is provided. The third section carefully derives the rotating frame for the basic model, and shows how to determine the frequencies and phases of the piecewise sinusoidal pulses which will be designed to generate any $S \in SU(4)$. The fourth section describes how to determine the amplitudes of these pulses and in the process explains how the two goals, $O_1$ and $O_2$ mentioned at the very beginning of this section, help in finding the amplitude and the duration of the pulses. Some conclusions are offered in the next section. An appendix describes how to go about calculating the Euler angle analogues for $SU(4)$. 


2 Review of Basic $SU(2)$ Facts

The Pauli matrices will be denoted as: $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

In terms of this definition of the Pauli matrices, a few important $4 \times 4$ Hermitian matrices can also be defined:

$$I_{1k} = \sigma_k \otimes I_2; I_{2k} = I_2 \otimes \sigma_k, \ k = x, y, z; \quad (2.3)$$

Note that both in the definition of the Pauli matrices and in the above equation, the customary factor of $\frac{1}{2}$ has been omitted. This is for notational convenience and does not affect any of the results below.

Next, a very useful representation of the $SU(2)$ matrices, the Cayley-Klein parametrization, follows.

$$S = S(\alpha, \zeta, \mu) = \begin{pmatrix} e^{i\zeta} \cos \alpha & e^{i\mu} \sin \alpha \\ e^{i(\pi-\mu)} \sin \alpha & e^{-i\zeta} \cos \alpha \end{pmatrix} \quad (2.4)$$

$\alpha, \zeta, \mu$ are the Cayley-Klein parameters of $S$. Since this parametrization is nothing but the entries of $S$ written in polar form, it is clear that $\zeta$ and $\mu$ may be taken to be in $[0, 2\pi)$ and $\alpha$ to be in $[0, \frac{\pi}{2}]$.

Crucial for the purposes of this paper is an Euler parametrization, in terms of $\sigma_x$ and $\sigma_y$, of any $S(\alpha, \zeta, \mu)$:

$$S(\alpha, \zeta, \mu) = e^{iD\sigma_x}e^{iE\sigma_y}e^{iF\sigma_x} \quad (2.5)$$

Though, in principle, the Euler angles $D, E$ and $F$ may be obtained from more common Euler angle parametrizations [23], an explicit formula for them in terms of the Cayley-Klein coordinates goes a long way towards making the techniques of this paper genuinely constructive. Therefore, the following relations are very useful, [24]:

$$\cos(E) = \sqrt{\cos^2 \zeta \cos^2 \alpha + \sin^2 \mu \sin^2 \alpha} \quad (2.6)$$
\[
\sin(D - F) = \frac{\sin \zeta \cos \alpha}{\sqrt{\sin^2 \zeta \cos^2 \alpha + \cos^2 \mu \sin^2 \alpha}} \quad (2.7)
\]
\[
\sin(D + F) = \frac{\sin \mu \cos \alpha}{\sqrt{\sin^2 \mu \sin^2 \alpha + \cos^2 \zeta \cos^2 \alpha}} \quad (2.8)
\]

The parameters, \(D, E\) and \(F\) can be assumed to be in \([0, 2\pi]\) if needed.

The next item on the list is the following decomposition of any matrix, \(S \in SU(4)\) into factors which are exponentials of \(I_{ij}, i = 1, 2, j = x, y\) and the matrix \(I_{1z}I_{2z}\) \([17]\).

\[
S = K_1 \otimes K_2 e^{-i\frac{\pi}{4}I_{1y}} e^{-i\frac{\pi}{4}I_{2y}} e^{-i\theta_I I_{1x}} I_{1z} e^{-i\frac{\pi}{4}I_{2x}} e^{-i\theta_I I_{1x}} I_{2z} e^{-i\theta_I I_{1z}} K_3 \otimes K_4 \quad (2.9)
\]

In \([23]\) the matrices \(K_i, i = 1, \ldots, 4\) are some matrices in \(SU(2)\). This decomposition follows from the well known fact that the Lie algebra \(su(2) \otimes su(2)\) and its orthogonal complement in the Lie algebra \(su(4)\) provide a Cartan decomposition of the Lie group \(SU(4), \ [15, 14, 16]\). In \([17]\) this fact and some calculations are used to obtain the decomposition \([23]\). Note, however that they do not provide any formulae for the \(K_i, i = 1, \ldots, 4\) and the \(\theta_k, k = 1, \ldots, 3\) in terms of the target matrix \(S\). In the appendix, we will ameliorate this problem. For the moment, however, expanding each of the \(K_i, i = 1, \ldots, 4\) into its \(\sigma_x, \sigma_y\) Euler angles via Equation \([2.6]\) and using some Kronecker calculus, leads to the following equation, which is the one we will work with:

\[
S = e^{iD_1 I_{1x}} e^{iE_1 I_{1y}} e^{iF_1 I_{1z}} e^{iD_2 I_{2x}} e^{iE_2 I_{2y}} e^{iF_2 I_{2z}} e^{-i\frac{\pi}{4}I_{1y}} e^{-i\frac{\pi}{4}I_{2y}} e^{-i\theta_I I_{1x}} I_{1z} I_{2z} \quad (2.10)
\]

The \((D_i, E_i, F_i)\) are the Euler angles of the \(K_i \in SU(2), i = 1, \ldots, 4\).

### 3 Determination of the Frequencies and Phases

Consider a pair of coupled spins in the weak coupling limit. The system is assumed to be heteronuclear, so that it is possible to address each spin individually as long the as the frequency of the corresponding field is resonant with the Larmor frequency of the spin, \(\omega_i\), in question and the field can be bounded in amplitude. Thus, the model is
\[ \dot{V} = -\frac{i}{2}(\dot{A}V + u_1(t)B_1V + u_2(t)B_2V), V \in SU(4) \]

where the internal Hamiltonian, \( \dot{A} \) is \( \omega_1 \sigma_z \otimes I_2 + \omega_2 I_2 \otimes \sigma_z + J \sigma_z \otimes \sigma_z \), and the interaction Hamiltonians are \( B_1 = b_1 \sigma_x \otimes I_2 \) and \( B_2 = b_1 \sigma_y \otimes I_2 \). The \( b_i, i = 1, 2 \) (\( b_2 \) appears below) are constants related to the gyromagnetic ratios, and the \( \omega_i, i = 1, 2 \) are the Larmor frequencies. Finally, \( u_1(t) \) and \( u_2(t) \) are sinusoidal fields to be designed:

\[ u_1(t) = c \cos(\omega t + \phi), u_2 = c \sin(\omega t + \phi) \quad (3.11) \]

The frequency, \( \omega \), will be taken to be \( \omega_1 \). So the design procedure amounts to specifying the amplitude, \( c \), the phase, \( \phi \) and the duration of the pulses. These will be chosen in a piecewise constant manner. The fourth section is essentially devoted to finding the amplitudes and the durations. How the phases ought to be chosen will become clear later in this section.

The above equation was derived assuming that the first spin was being addressed. If the second spin is being addressed, then \( B_1, B_2 \) would be replaced by \( b_2 I_2 \otimes \sigma_x \) and \( b_2 I_2 \otimes \sigma_y \) respectively, while the frequency, \( \omega \), of the field would be replaced by \( \omega_2 \).

Let us now derive the rotating frame in which the problem of preparation of a target will be translated into finding piecewise constant controls for an associated system in the rotating frame (see [25] for related considerations). Set

\[ U(t) = e^{tF}V(t) \]

with

\[ F = \frac{i}{2}(\omega_2 I_2 \otimes \sigma_z + \omega_1 \sigma_z \otimes I_2) \]

Then a few calculations reveal that

\[ \dot{U} = -\frac{i}{2}(J_{1z} I_2)U - \frac{i}{2}(c_b \Delta \otimes I_2)U \quad (3.12) \]

where

\[
\Delta = \begin{pmatrix}
0 & e^{-i\phi} \\
e^{i\phi} & 0
\end{pmatrix}
\]
Note that the matrix $\Delta$ is independent of time and is parametrized by the phase, $\phi$, of the field which can be chosen. Thus, if we choose $\phi = 0$, $\Delta$ is $\sigma_x$ and if we set $\phi = \frac{\pi}{2}$, $\Delta$ is $\sigma_y$.

A similar calculation reveals that the same rotating frame can be used to address the other spin (with the frequency of the field, $\omega = \gamma_2$) to obtain the following equation

$$
\dot{U} = -\frac{i}{2}(JI_1 I_2 z - (cb_2 I_2 \otimes \Delta))U
$$

(3.13)

Once again by choosing the phase, $\phi$, one can ensure that $\Delta$ is either $\sigma_y$ or $\sigma_x$.

The upshot of the foregoing is that by choosing the frequency of the field to be resonant with one of the spins and by choosing the phase in an appropriate manner, passage to a unique rotating frame leads to the following system, which is controlled by constant inputs:

$$
\dot{U} = -\frac{i}{2}AU - \frac{i}{2}dBU, U(0) = I_4
$$

(3.14)

with $A = J\sigma_z \otimes \sigma_z$ and $B$ one of the matrices $I_{1x}, I_{2x}, I_{1y}, I_{2y}$ where $I_{ij} = \sigma_j \otimes I_2, j = x, y$ and $I_{2j} = I_2 \otimes \sigma_j, j = x, y$. The constant, $d$, is related to the amplitude of the field and other constants of the system. This is useful because the Cartan decomposition, i.e., Equation (2.10) of Section 2, consists precisely of the exponentials of one of $A, I_{ij}, i = 1, 2, j = x, y$. Thus, if the exponential of a certain $I_{ij}$ is required we choose the frequency and phase of the field so that $B$ of Equation (4.15) becomes $I_{ij}$, and then follow the procedure in the next section to determine, $d$ (hence, the amplitude of the field).

It is interesting to observe that while in the rotating frame, we are exciting one spin with one of the $x$ or $y$ magnetic field components, in the original frame we are exciting any one spin by using both the $x$ and $y$ magnetic field components.

4 Determining the Amplitudes

The basic model derived in the previous section leads to the following system in the rotating frame, for which we will design piecewise constant controls:

$$
\dot{U} = -iAU - iu(t)BU, U(0) = I_4
$$

(4.15)
where \( A = I_1 z I_2 z = \sigma_z \otimes \sigma_z \), and \( B \) is one of the \( I_{ij}, i = 1, 2, j = x, y \) and \( u(t) \) the control (to be determined) is piecewise constant.

Note, for the sake of easy bookkeeping, the constants \( J, b, i \) have been dropped in Equation (4.13). However, once results for the above model are available it is a routine matter to derive results for the actual model, with these parameters present.

Going back to the equation (2.10) it is clear that factors which are the exponentials of \(-iA\) can be generated by free evolution i.e., by setting \( u(t) = 0 \) for an amount of time given by the corresponding \( \theta_k \). Indeed, \( e^{-i\theta_k A} \) is a diagonal matrix, \( \text{diag}(e^{-i\theta_k}, e^{i\theta_k}, e^{i\theta_k}, e^{-i\theta_k}) \). If \( \theta_k \geq 0 \), then \( e^{-i\theta_k A} \) can be prepared by free evolution for \( \theta_k \) units of time. If \( \theta_k < 0 \) then, \( e^{-i\theta_k A} \) can be prepared by free evolution for \( 2\pi + \theta \) units of time. Only for free evolution terms are periodicity arguments resorted to. For other factors, instead of resorting to periodicity arguments, substantial use of the structure of the drift \(-iA\) will be made.

So all that remains to be addressed is preparing factors which are exponentials of the \(-iI_{ij}\) via controlled pulses. In other words, the main goal at this stage is to decompose the exponential, \( e^{-iLI_{ij}}, i = 1, 2, j = x, y \), for any \( L \in R \), as:

\[
e^{-iLI_{ij}} = \prod_{k=1}^{Q} e^{(-ia_k A - ib_k I_{ij})}, i = 1, 2, j = x, y, A = I_1 z I_2 z
\]  

(4.16)
satisfying i) \( O_1 \) \( a_k > 0, k = 1, \ldots, Q \) and ii) \( O_2 \) \( |b_k| \leq C, k = 1, \ldots, Q \). Constructive methods for obtaining the desired \( a_k, b_k \) in terms of \( S \) will be provided. At this stage the formulae for the \( a_k, b_k \) will be provided in terms of the parameters, \((D_i, E_i, F_i), i = 1, \ldots, 4\) and \( \theta_k, k = 1, \ldots, 3 \) of Equation (2.10). The appendix indicates a procedure which obtains these \( SU(4) \) “Euler angles” directly from the entries of \( S \). Note that \( a_k \) is the duration of the \( k \)th pulse and \( \frac{b_k}{a_k} \) is its amplitude. The basic strategy is to first achieve \( O_1 \) and then constructively modify the resulting decomposition to meet \( O_2 \) also. The proof below shows how achieving \( O_2 \) leads also to arbitrarily bounding the amplitude of the pulse.

Theorem 4.1 The matrix \( \exp(-iLI_{1z}), L \in R \) can be factored explicitly as \( \prod_{k=1}^{Q} \exp(-ia_k A - \ldots) \)
ib_1I_{1x})$ with $A = I_{1z}I_{2z}$ and with $a_k > 0, k = 1, \ldots, 3$ and $b_1 = 0 = b_3$, if $\cos L \neq 0$. If $\cos L = 0$, then four factors are needed, with $b_1 = 0 = b_4$. Further, this factorization can be refined constructively, by increasing the number of factors, to ensure that $|b_k| \leq C, k = 1, \ldots, Q$. This decomposition can be further refined to meet the condition, $|\frac{a_k}{\lambda_k}| \leq D$, for any prescribed $D > 0$. Similar statements hold for the exponentials of $I_{2z}, I_{1y}$ and $I_{2y}$ with the matrix for appropriately different sets of $a_k$’s and $b_k$.

**Proof:** The proof will be given only for the exponential of $\exp(-iLI_{1x})$, since the proof for the others are very similar.

The special structure of $I_{1z}I_{2z}$ and $I_{1x}$ results in the following matrix for $\exp(-ia_kA - ib_kI_{1x})$

$$
\begin{pmatrix}
\cos \lambda_k - \frac{ib}{\lambda_k} a_k \sin \lambda_k & 0 & -\frac{ib}{\lambda_k} \sin \lambda_k & 0 \\
0 & \cos \lambda_k + \frac{i}{\lambda_k} a_k \sin \lambda_k & 0 & -\frac{ib}{\lambda_k} \sin \lambda_k \\
-\frac{ib}{\lambda_k} \sin \lambda_k & 0 & \cos \lambda_k - \frac{i}{\lambda_k} a_k \sin \lambda_k & 0 \\
0 & -\frac{ib}{\lambda_k} \sin \lambda_k & 0 & \cos \lambda_k - \frac{i}{\lambda_k} a_k \sin \lambda_k
\end{pmatrix}
$$

(4.17)

where $\lambda_k = \sqrt{(a_k^2 + b_k^2)}$. In particular, setting $a_k = 0$ and $b_k = L$ yields the exponential of $-iLI_{1x}$. Similarly, an explicit calculation yields the following formula:

$$
\exp(-iL\sigma_y \otimes \sigma_z) =
\begin{pmatrix}
\cos L & 0 & \sin L & 0 \\
0 & \cos L & 0 & -\sin L \\
-\sin L & 0 & \cos L & 0 \\
0 & \sin L & 0 & \cos L
\end{pmatrix}
$$

(4.18)

Using the last two formulae, the following useful identity is obtained:

$$
\exp(-iLI_{1x}) = \exp(-i\frac{7\pi}{4}I_{1z}I_{2z})\exp(-iL\sigma_y \otimes \sigma_z)\exp(-i\frac{\pi}{4}I_{1z}I_{2z})
$$

(4.19)

Thus, to prepare the matrix $\exp(-iLI_{1x})$, free evolution for $\frac{7\pi}{4}$ units of time for the first factor above is used and free evolution for $\frac{\pi}{4}$ units of time for the third factor is used. Therefore, it remains to produce the middle factor, $\exp(-iL\sigma_y \otimes \sigma_z)$ via controlled pulses. Since, the matrix $-iL\sigma_y \otimes \sigma_z$ is, up to a constant, the commutator of $A$ and $B_1$, it seems
plausible that its exponential can be represented as a product, \( \Pi_{k=1}^{2} \exp[-i(a_{k}I_{1z}I_{2z} + b_{k}I_{1z})] \).

To demonstrate this, three cases need to be considered: i) \( \cos L > 0 \), ii) \( \cos L < 0 \) and iii) \( \cos L = 0 \).

**The Case** \( \cos L > 0 \): Evaluating the product \( \Pi_{k=1}^{2} \exp[-i(a_{k}I_{1z}I_{2z} + b_{k}I_{1z})] \) and choosing \( \lambda_{1} = \sqrt{a_{1}^{2} + b_{1}^{2}} = \frac{3\pi}{2} \) and \( \lambda_{2} = \sqrt{a_{2}^{2} + b_{2}^{2}} = \frac{\pi}{2} \) and equating the result to the matrix \( \exp(-iL\sigma_{y} \otimes \sigma_{z}) \) leads to the following equations:

\[
\frac{a_{1}a_{2} + b_{1}b_{2}}{\lambda_{1}\lambda_{2}} = \cos L \\
\frac{a_{1}b_{2} - a_{2}b_{1}}{\lambda_{1}\lambda_{2}} = -\sin L
\]

These two equations can be solved as follows. Choose \( b_{1} = 0, a_{1} = \frac{3\pi}{2}, b_{2} = -\frac{\pi}{2} \sin L, a_{2} = \frac{\pi}{2} \cos L \). Thus, \( O1 \) has been met for the case that \( \cos L > 0 \).

**The Case** \( \cos L < 0 \): Now choose \( \lambda_{1} = \frac{\pi}{2} \) and \( \lambda_{2} = \frac{\pi}{2} \). The resulting set of equations has the following solution: \( b_{1} = -\frac{\pi}{2} \sin L, a_{1} = -\frac{\pi}{2} \cos L, a_{2} = \frac{\pi}{2} \) and \( b_{2} = 0 \). Thus, \( O1 \) has been achieved for this case also.

**The Case** \( \cos L = 0 \): Now choose \( \lambda_{1} = \frac{\pi}{2} \) and \( \lambda_{2} = \frac{\pi}{2} \). Then, the equations to solve become

\[
\frac{a_{1}a_{2} + b_{1}b_{2}}{\lambda_{1}\lambda_{2}} = 0 \quad \text{and} \quad \frac{a_{1}b_{2} - a_{2}b_{1}}{\lambda_{1}\lambda_{2}} = (-1) \sin(L). \]

If \( \sin(L) = 1 \), choose \( a_{1} = \frac{1}{\sqrt{2}} \lambda_{1} \) and \( a_{2} = \frac{1}{\sqrt{2}} \lambda_{2} \), and \( b_{1} = -a_{1} \) and \( b_{2} = a_{2} \). If \( \sin(L) = -1 \), then choose \( a_{1} = \frac{1}{\sqrt{2}} \lambda_{1}, a_{2} = \frac{1}{\sqrt{2}} \lambda_{2}, \) and \( b_{1} = a_{1} \) and \( b_{2} = -a_{2} \).

Now concatenating the pulses which prepare \( \exp(-iL\sigma_{y} \otimes \sigma_{z}) \) with the free evolution terms which prepare \( \exp(-i\frac{\pi}{4}\sigma_{y} \otimes \sigma_{z}) \) and \( \exp(-i\frac{\pi}{4}\sigma_{z} \otimes \sigma_{z}) \) yields the stated values for the number of factors for \( O1 \).

To meet \( O2 \), notice only the \( e^{-iL\sigma_{y} \otimes \sigma_{z}} \) term needs to be addressed, since the others are free evolution terms and hence have pulse area equal to 0. Even in the preparation of the \( e^{-iL\sigma_{y} \otimes \sigma_{z}} \) term, there is only one term which is not a free evolution term (except when \( \cos L = 0 \)). The corresponding, \( \mid b_{k} \mid \) is exactly equal to \( \frac{\pi}{2} \mid \sin L \mid \). So to meet \( O2 \), \( \theta \) has to be such that \( \mid \sin L \mid \leq C \frac{\pi}{2} \). This amounts to requiring that \( L \) be within a prescribed bound of 0. If \( L \) is not already of the form, then we factor \( e^{iL_{1z}} \) as \( \Pi_{k=1}^{L} e^{iL_{k}I_{1z}} \) with the \( L_{k} \) satisfying the required deviation from 0 condition. Clearly this can always be
done.

Notice further, that this process of meeting $O_2$ also ensures that the amplitude of the pulse, $| \frac{b_k}{a_k} |$ can also be bounded arbitrarily. Indeed, the amplitude of the pulses are either 0 (corresponding to free evolution terms) or $| \tan L |$. Clearly any process which ensures that $| \sin L |$ is within a prescribed bound can ensure the same for $| \tan L |$.

If $\cos L = 0$, then write $\exp(-iLI_{1x})$ as $(\exp(-i\frac{L}{2}I_{1x}))^2$, and proceed as in the $\cos L \neq 0$ cases. This finishes the construction.

**Remark 4.1** The values obtained for $a_k$ and $b_k$ are certainly not the only possibilities. Since one of the principal goals of this paper is to show that the pulse amplitudes can be arbitrarily bounded, the $a_k$ and $b_k$ satisfying $O_1$ were so chosen that the resulting decomposition could be modified with minimal fuss, to meet $O_2$. This means that the proof chosen was biased towards free evolution terms. In practice, of course one can find other values so that the cumulative time taken can also be kept within reasonable bounds.

**Remark 4.2** Suppose $S$ is prepared in the rotating frame in $T_S$ units of time. Then in the original coordinates the matrix $e^{-T_SF}S$ has been prepared. Depending on the system, it may be desirable to rectify this error. Since, $T_S \geq \sum_{k=1}^3 \theta_k$ [with $\theta_k$ given in Equation (1.2)], this problem cannot be wished away by hard pulses. Of course, hard pulses can be further used to generate $e^{T_SF}$. However, this introduces further inaccuracies in addition to those caused by the use of hard pulses to prepare $S$ in the rotating frame. We suggest two methods which do not need hard pulses to rectify this deviation. The first is to prepare $e^{T_0F}S$ by soft pulses in the rotating frame for a real parameter, $T_0$, to be chosen such that the time, $T_1$, to prepare $e^{T_0F}$ in the rotating frame, satisfies $T_1 + T_S = T_0$. This leads to a transcendental equation for $T_0$ [specifically, $\frac{1}{\sqrt{2}}[(\frac{21}{2} + \frac{1}{\sqrt{2}})\pi + T_S] = T_0 - \frac{1}{\sqrt{2}}(\cos \omega_1 T_0 + \cos \omega_2 T_0)]$. This has to be solved numerically. The second method is to use optimal control to drive the system, in the original coordinates, from $I_4$ to $e^{T_SF}$, with a quadratic cost functional incorporating bounds on the field fluence and deviation of the state from the target. The fact that the target state, $e^{T_SF}$ is diagonal will help reduce the complexity of optimal control calculations.
5 Conclusions

In this paper, a constructive procedure for generating a desired unitary generator in $SU(4)$, via the control of a coupled, heteronuclear, two spin system was described. The sinusoidal pulses that were produced were not hard pulses, but instead could be bounded both in amplitude and pulse area.

An interesting problem is to investigate the methodology of this paper for systems which are not studied by addressing individual spins selectively. It is relatively straightforward to see that an analogous Cartan decomposition can be modified to express every target $S$ in a manner analogous to Equation (1.2). However, the remaining calculations seem to require new methods. Investigation of this problem will be a worthwhile research problem.

6 Appendix: Determining the Euler Parameters for $SU(4)$

To make the methodology proposed here (or for that matter any methodology based on the Cartan decompositions) genuinely constructive, it is extremely desirable to find the fifteen parameters, $(D_i, E_i, F_i), i = 1, \ldots, 4$ and $\theta_k, k = 1, \ldots, 3$ of Equation (2.10), as explicitly as possible, in terms of the entries of the target matrix $S \in SU(4)$. In principle, this amounts to solving sixteen equations for fifteen unknowns. However, this is not really a satisfactory state of affairs. To make the point further clear, consider determining the Euler angles of an $SU(2)$ matrix in closed form in terms of the entries of the matrix. This is principally facilitated by the availability of the Cayley-Klein representation, i.e., Equation (2.4). A similar representation for $SU(4)$ matrices is not available in the literature, and thus the resulting system of equations cannot even be written down in a manner which will facilitate investigating the possibility of a closed form determination of the $D_i, E_i, F_i, i = 1, \ldots, 4$ and the $\theta_k, k = 1, \ldots, 3$.

Therefore, we eschew working directly with $S$ itself. Instead, $S$ will be first decomposed
into a product of matrices, each of which has a simpler structure, so that finding these fifteen parameters for each of these factors is more tractable. Note that strictly speaking, this will not result in a factorization of the form in Equation (2.11) for the original matrix $S$, since now the factors of each of the $S_i$ become intertwined. However, it will produce a factorization of the form in Equation (1.2). But, this is all that is needed to achieve the constructive generation of $S$.

The main idea is to write $S = \prod_{i=1}^{Q} S_i$ so that each of the $S_i$ can be expressed solely in terms of a single $SU(2)$ matrix. While, this may mean that the number of parameters (and, thus the number of control pulses) needed are larger than what would result if the fifteen parameters were directly determined for $S$, it has the advantage that close to explicit formulae can be produced for the Euler angles, whereas (pending further investigation) there is nothing remotely close to explicit when working with $S$ itself. Furthermore, as will be clear soon, many of the $K_k, k = 1, \ldots, 4$ turn out to be $I_2$ for many of the factors $S_i$, and likewise many of the $\theta_k$ are zero. Thus, the number of factors and pulses is not all that high.

The decomposition that will be used is the standard Givens decomposition, [26, 27], modified slightly for the problem at hand. The usual Givens decomposition is produced as follows. Premultiply $S^\dagger$, the inverse of $S$, by a sequence of matrices, $S_i$, which successively reduce the columns of $S$ to the unit vectors, $e_i$, i.e., the fourth column is reduced to $(0, 0, 0, 1)$ and the third to $(0, 0, 1, 0)$ etc., Then it can be shown that $Q = 6$, [8], and thus

$$S = \prod_{i=1}^{6} S_i$$

Usually these $S_i$ are taken to be a matrix, which upto permutation of rows and columns, is a block matrix consisting of $I_2$ and an explicitly determined $SU(2)$ matrix. Here, we will make a slight modification, we will take $S_6$ to be a tensor product of two $SU(2)$ matrices. The remaining five will be, upto permutation, block matrices with blocks equal to $I_2$ and a specific $SU(2)$ matrix.

To briefly illustrate the structure of $S_6$ (the remaining $S_k$ are constructed in the manner described in [8]), suppose that Suppose $S^\dagger = \text{col}(a, b, c, d)$ (thus $a, b, c, d$ are the four
columns of $S^\dagger$).

Then choose $S_6 = e^{i\pi v} \otimes S(\alpha_6, \zeta_6, \mu_6)$ where $S(\alpha_6, \zeta_6, \mu_6)$ is the unique $SU(2)$ matrix which takes the vector $(d_1, d_2)$ to the vector $(||d_1, d_2||, 0)$. Note that once $d_1, d_2$ are known one can explicitly write down this $SU(2)$ matrix (here use is being made of the fact that given any two points on a sphere of any radius in $C^2$ there is a unique $SU(2)$ matrix which conveys the first to the second and that this matrix can be found explicitly).

The remaining, $S_k$ have the following structure.

\[
S_5 = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & \cos \alpha_5 e^{i\zeta_5} & \sin \alpha_5 e^{i\mu_5} \\
0 & 0 & \sin \alpha_5 e^{i(\pi - \mu_5)} & \cos \alpha_5 e^{-i\zeta_5}
\end{pmatrix}
\]

\[
S_4 = \begin{pmatrix}
\cos \alpha_4 e^{i\zeta_4} & 0 & 0 & \sin \alpha_4 e^{i\mu_4} \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
\sin \alpha_4 e^{i(\pi - \mu_4)} & 0 & 0 & \cos \alpha_4 e^{-i\zeta_4}
\end{pmatrix}
\]

\[
S_3 = \begin{pmatrix}
\cos \alpha_3 e^{i\zeta_3} & \sin \alpha_3 e^{i\mu_3} & 0 & 0 \\
\sin \alpha_3 e^{i(\pi - \mu_3)} & \cos \alpha_3 e^{-i\zeta_3} & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

\[
S_2 = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \alpha_2 e^{i\zeta_2} & \sin \alpha_2 e^{i\mu_2} & 0 \\
0 & \sin \alpha_2 e^{i(\pi - \mu_2)} & \cos \alpha_2 e^{-i\zeta_2} & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

and

\[
S_1 = \begin{pmatrix}
\cos \alpha_1 e^{i\zeta_1} & \sin \alpha_1 e^{i\mu_1} & 0 & 0 \\
\sin \alpha_1 e^{i(\pi - \mu_1)} & \cos \alpha_1 e^{-i\zeta_1} & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]
Once again each of the SU(2) matrices, \( S(\alpha_k, \zeta_k, \mu_k) \), \( k = 1, \ldots, 5 \), can be constructively determined from the entries of \( S \).

Now let us determine the fifteen Euler angles for the matrices \( S_i, i = 1, \ldots, 6 \). Since, the \( S_i \) are significantly simpler than the matrix, \( S \), this is a more tractable task. In what follows the matrices \( K_k, i = 1, \ldots, 4 \) and the real constants, \( \theta_k, k = 1, \ldots, 3 \) will be described for each of the \( S_i, i = 1, \ldots, 6 \). Once the \( K_k \) are known, it is easy to find the \( \sigma_x, \sigma_y \) Euler angles, \( (D_k, E_k, F_k) \), by using Equation (2.6). Therefore, that step will not be executed here.

To simplify notation, three real parameters \( P, Q \) and \( R \) are introduced. They are related to the parameters \( \theta_k, k = 1, \ldots, 3 \) by:

\[
P = \frac{\theta_1 - \theta_2}{4}, \quad Q = \frac{\theta_3}{4}, \quad R = \frac{\theta_1 + \theta_2}{4}
\]

(6.20)

Below, the values of \( P, Q \) and \( R \) for the \( S_i, i = 1, \ldots, 6 \) will be given. Obtaining the \( \theta_k, k = 1, \ldots, 3 \) is then routine.

\( S_6 \): Clearly, \( S_6 = K_1 \otimes K_2 \), where \( K_1 = e^{\frac{i}{2} \pi I_y} \) and \( K_2 = e^{iD_6 \sigma_x} e^{-iE_6 \sigma_y} e^{-iF_6 \sigma_z} \). The Euler angles \( (D_6, E_6, F_6) \) are the Euler angles of the matrix \( S(\alpha_6, \zeta_6, \mu_6) \) determined according to Equation (2.7). The matrices \( K_3, K_4 \) can be taken to be \( I_2 \) and the constants, \( P, Q \) and \( R \) (and hence the \( \theta_k, k = 1, 2, 3 \) can be set equal to zero.

\( S_5, S_1 \) and \( S_3 \): The matrices \( S_1 \) and \( S_3 \) are essentially the same in structure, and they are analogous to \( S_5 \). Thus, calculations for \( S_5 \) will be shown here and the modifications required for \( S_1 \) and \( S_3 \) will be given.

So consider determining the fifteen Euler parameters of \( S_5 \).

Pick \( K_1 = I_2 \) and \( K_2 = S(\alpha, \zeta, \mu) \) where the parameters \( (\alpha, \zeta, \mu) \) will be presently determined. Choose \( P \) an \( R \) equal to zero (thus \( \alpha_1 = 0 = \alpha_2 \)). Multiplying out all but
the factors $K_3 \otimes K_4$, leads to the following matrix:

\[
\begin{pmatrix}
\cos \alpha e^{i(\zeta - Q)} & \sin \alpha e^{i(\mu + Q)} & 0 & 0 \\
\sin \alpha e^{i(\pi - \mu - Q)} & \cos \alpha e^{-i(Q - \zeta)} & 0 & 0 \\
0 & 0 & \cos \alpha e^{i(Q + \zeta)} & \sin \alpha e^{i(\mu - Q)} \\
0 & 0 & \sin \alpha e^{i(\pi - \mu + Q)} & \cos \alpha e^{-i(Q + \zeta)}
\end{pmatrix}
\]

Now choose $K_3 = I_2$ and $K_4$ to be the inverse of the top left hand block of the last matrix (note since the matrix in question is in $SU(2)$ it is very straightforward to find its inverse).

This then means that the matrix $S(\alpha_5, \zeta_5, \mu_5)$ (which is known) should equal the matrix:

\[
\begin{pmatrix}
\cos^2 \alpha e^{i2Q} + \sin^2 \alpha e^{i2Q} & \cos \alpha \sin \alpha \left(e^{i(2Q + \mu + \zeta - \pi)} + e^{i(\mu + \zeta - 2Q)}\right) \\
\cos \alpha \sin \alpha \left(e^{i(\pi - \mu - \zeta + 2Q)} + e^{-i2Q}\right) & \sin^2 \alpha e^{i2Q} + \cos^2 \alpha e^{-i2Q}
\end{pmatrix}
\]

We will find $\alpha, \zeta, \mu$ and $Q$ (and hence $\alpha_3 = 4Q$) by equating the top row of the two matrices in the last equation (since both the matrices are in $SU(2)$, this will automatically mean that the second row of the two are the same). This leads to the equations:

\[
\sqrt{\cos^2 2Q + \cos^2 \alpha \sin^2 2Q} = \cos \alpha_5 \\
- \cos 2\alpha \tan 2Q = \tan \zeta_5 \\
\left(- \frac{\cos(\mu + \zeta)}{\sin(\mu + \zeta)}\right) = \tan \mu_5
\]

In the above system of equations, the unknowns are $\alpha, \zeta, \mu$ and $Q$, and the known variables are $\alpha_5, \zeta_5, \mu_5$. Thus, we have three transcendental equations for four unknowns. Thus, there will be in general many solutions. Notice, that the first two equations involve only two of the unknowns, viz., $\alpha$ and $Q$, and thus it is this pair of equations which will have to be solved numerically. The one parameter family of freedom comes from the third equation, where there are two unknowns.

In summary, the Euler angles of $S_5$ have been determined. The Euler angles of $S_3$ (and, thus $S_1$) can also be determined via a similar technique. Indeed, the calculations are similar to those for $S_3$ except that $K_4$ will be taken to be the inverse of the $SU(2)$ matrix in the bottom block of the matrix resulting from multiplying all but the last six factors of Equation (2.10).
**S$_2$ and S$_4$:** The matrices $S_4$ and $S_2$ bear a resemblance to one another. Calculations for $S_2$ will be shown together with the modifications needed for the $S_4$ case.

Choose $K_1 = e^{i\eta_1 \sigma_z}$, $K_2 = e^{i\eta_2 \sigma_z}$, $K_3 = I_2$ and $K_4 = e^{i\eta_3 \sigma_z}$, for some real numbers $\eta_k, k = 1, \ldots, 3$ to be determined shortly. Choose $Q = 0$ and $P = 0$ and $R = \alpha_2$ (where $\alpha_2$ is a Cayley-Klein parameter of $S_2 = S(\alpha_2, \zeta_2, \mu_2)$, and thus, is known beforehand).

The parameters $\eta_k, k = 1, \ldots, 3$ are found by solving the linear system of equations:

\[
\begin{align*}
\eta_1 + \eta_2 + \eta_3 &= 0 \\
\eta_1 - \eta_2 + \eta_3 &= \zeta_2 \\
\eta_1 - \eta_2 - \eta_3 &= \mu_2 + \frac{\pi}{2}
\end{align*}
\]

For $S_4$ the only modification needed in this procedure is that $R = 0$ and $P = \alpha_4$.

This completes the determination of the fifteen, $SU(4)$, “Euler” angles for each of the matrices $S_i, i = 1, \ldots, 6$ in the specially chosen Givens decomposition of the given target $S \in SU(4)$.

**Remark 6.1** There is considerable liberty in the Givens decomposition. For instance, the order in which the columns are reduced to the corresponding unit vectors is one such degree of freedom. The factors that were chosen above were expressly intended to facilitate the calculation of the corresponding fifteen $SU(4)$ angles. It is an interesting problem to find other factorizations which yield different values of the $t_k$ in Equation (1.2).

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