The Optimal Control Problem on $SO(4)$ and its Applications to Quantum Control

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Abstract

In this paper, we consider the problem of steering control via an input electro-magnetic field for a system of two interacting spin $\frac{1}{2}$ particles. This model is of interest in applications because it is used to perform logic operations in quantum computing that involve two quantum bits. The describing model is a bilinear system whose state varies on the Lie group of special unitary matrices of dimension 4, $SU(4)$. By using decompositions of the latter Lie group, the problem can be decomposed into a number of subproblems for a system whose state varies on the (smaller) Lie group of $4 \times 4$ proper orthogonal matrices, $SO(4)$. We tackle the time optimal control problem for this system and show that the extremals can be computed explicitly and they are the superposition of a constant field and a sinusoidal one.

Keywords: Control of quantum mechanical systems, Optimal control, Particles with spin, Decompositions of Lie Groups.

1 Introduction and Motivation

The goal of this paper is to present an algorithm for the control of two interacting spin $\frac{1}{2}$ particles in an electro-magnetic field. This system is important because it is used in implementations of quantum computers [10] to perform operations on two quantum bits (the states of the two spin $\frac{1}{2}$ particles). This system is also of interest in nuclear magnetic resonance spectroscopy and, more in general, it is a prototypical system in quantum control theory, being the next more difficult case after the well studied two level case [5], [9], [24]. The
algorithm we present in this paper allows to drive the state of this system to any desired final state with arbitrary accuracy, by prescribing an appropriate time varying electro-magnetic field. We use Lie group decompositions, such as the ones described in [14] and [23], to reduce the problem to a control problem on the Lie group $SO(4)$. The time optimal control problem for a system whose state varies on $SO(4)$ is then tackled. We obtain a complete classification of normal and abnormal extremals and show how the optimal control functions can be computed explicitly. The consideration of the time as the cost in the control of quantum mechanical systems is quite natural in that, in this context, one would like to obtain the fastest state transfer in order to prevent decoherence to set in. Only slight modifications are necessary to handle the case where the cost is an energy-type, quadratic in the control, cost functional and one can prove that the extremals have the same form in this case.

The Hamiltonian we will consider for a system of two spin $\frac{1}{2}$ particles, which interact with each-other, and are immersed in an electro-magnetic field, is given by (see e.g. [11] and [13])

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

The two terms on the right hand side of (1) represent the interaction of the two particles with the external electro-magnetic field (first term) and the interaction of the two particles with each-other (second term). In the first term, $u_{x,y,z}$ represents the $x$, $y$ and $z$ component of the field. We assume that we can vary all of the components of the input field. We assume that the system, which is typically an ensemble of identical spin systems, has been previously prepared in an (almost) pure state [25], for example by applying a constant magnetic field in the $z$ direction. $\gamma_1$ and $\gamma_2$ are the gyromagnetic ratios of particle 1 and 2, respectively. We will assume them to be different in this paper. The constant $J$ is the coupling constant between the two particles. The interaction is modeled with an isotropic term as opposed to the more general term $aI_{1x}I_{2x} + bI_{1y}I_{2y} + cI_{1z}I_{2z}$, however most of the results in the following will remain unchanged with the more general model. For $k = x, y, z$, we have

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

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

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

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. With the Hamiltonian in (1), one can write the time varying Schrödinger equation for the evolution operator $X$

$$i\hbar \dot{X} = H(t)X.$$
matrix representative of the identity operator 1 is the $2 \times 2$ identity matrix. Using (5) and (1), the resulting differential equation for the evolution operator $X$ has the form,

$$\dot{X} = \bar{A}X + \bar{B}_x X \bar{u}_x + \bar{B}_y X \bar{u}_y + \bar{B}_z X \bar{u}_z.$$  

(6)

The matrices $\bar{A}$, $\bar{B}_x$, $\bar{B}_y$ and $\bar{B}_z$ are $4 \times 4$ skew-Hermitian matrices with zero trace, namely matrices in $su(4)$. The solution of (6) has to be considered with initial condition equal to the identity $I_{4 \times 4}$, and varies on the Lie group of special unitary matrices of dimension $4 \times 4$, $SU(4)$.

The control problem we will consider for system (6) is a *steering problem*. We want to find control functions $\bar{u}_x$, $\bar{u}_y$, $\bar{u}_z$, to steer the state $X$ to a desired value in $SU(4)$. Similar steering problems on Lie groups have been considered in the literature on Geometric Control and its applications to Classical Mechanics. The papers [3], [19], [20]-[22], [26], [27], [29], and the books [15], [16], deal with problems and techniques related to the ones considered in the present paper.

The model in (6) can be simplified by normalizing the time and the control variables $\bar{u}_x$, $\bar{u}_y$, $\bar{u}_z$, so that the only parameter appearing in the equations is $r := \frac{\gamma_2}{\gamma_1}$. Moreover one can make a change of coordinates in equation (6) so as to diagonalize the matrix $\bar{A}$. The details of these manipulations are presented in [8]. The final result is an equation of the form

$$\dot{X} = AX + B_x Xu_x + B_y Xu_y + B_z Xu_z,$$  

(7)

where $u_x$, $u_y$, and $u_z$ represent the control variables and the matrices $A$, $B_x$, $B_y$, $B_z$, are given by

$$A := \text{diag}(3i, -i, -i, -i),$$  

(8)

$$B_x := \begin{pmatrix} 0 & 0 & 0 & r-1 \\ 0 & 0 & -(1+r) & 0 \\ 0 & 1+r & 0 & 0 \\ 1-r & 0 & 0 & 0 \end{pmatrix},$$  

(9)

$$B_y := \begin{pmatrix} 0 & 0 & r-1 & 0 \\ 0 & 0 & 0 & r+1 \\ 1-r & 0 & 0 & 0 \\ 0 & -1-r & 0 & 0 \end{pmatrix},$$  

(10)

$$B_z := \begin{pmatrix} 0 & r-1 & 0 & 0 \\ 1-r & 0 & 0 & 0 \\ 0 & 0 & 0 & -(1+r) \\ 0 & 0 & 1+r & 0 \end{pmatrix}.$$  

(11)

This form of Schrödinger equation is related to an important feature of the Lie algebra $su(4)$. This Lie algebra has the vector space decomposition

$$su(4) = S \oplus so(4),$$  

(12)
where $S$ is the vector space over the reals of symmetric, purely imaginary, zero trace, $4 \times 4$ matrices. The matrices $B_x$, $B_y$, $B_z$, with $r \neq 1$ generate all of $so(4)$ and $A \in S$. That this fact is useful for the control of system (7) has been recognized independently in the papers [6] and [18]. In particular, the paper [18] is closely related to the present paper since it deals with the time optimal problem for system (7) without assuming any bound on the magnitude of the control. In the spirit of [6] [18], the strategy in the present paper is to solve the control problem on $SO(4)$ first, by considering the driftless system

$$
\dot{X} = B_x Xu_x + B_y Xu_y + B_z Xu_z,
$$

(13)

and then to exploit the interaction to obtain the control over the whole group $SU(4)$.

The remainder of the paper is organized as follows. In Section 2, we show that every control strategy for system (13) can be used, along with a Lie group decomposition of $SU(4)$, to obtain control (with arbitrary degree of accuracy) to any element of $SU(4)$ for system (7). This motivates the investigation in the remaining sections in which we look for control algorithms for system (13). These control algorithms have to give a fast state transfer. The time optimal control problem for (13) is formalized in Section 3. In this Section, we also recall some basic results concerning existence of a solution to the optimal control problem and application of the Pontryagin maximum principle. In Section 4, we tackle this problem and give a complete classification of normal and abnormal extremals. The calculation of the optimal controls is discussed in Section 5. Some concluding remarks are presented in Section 6.

2 Lie group decompositions of $SU(4)$ and control on $SO(4)$

Given a target desired final condition $U_f$, the first step to drive the state of system (7) to $U_f$ is to decompose $U_f$ into the product of a number of factors belonging alternatively to $SO(4)$ and the one-dimensional subgroup corresponding to the matrix $A$. One possibility is described in the following Lemma.

**Lemma 2.1** Every matrix $U_f$ in $SU(4)$ can be written as

$$
U_f = K_4 e^{At_3} K_3 e^{At_2} K_2 e^{At_1} K_1,
$$

(14)

with $t_1, t_2, t_3 \geq 0$, $A$ given in (8), and $K_{1,2,3,4}$ matrices in $SO(4)$.

**Proof.** The decomposition of $su(4)$ in (12) is a Cartan decomposition (see e.g. [14]) and therefore every matrix $U_f \in SU(4)$ can be written as

$$
U_f = K_1 FK_2,
$$

(15)

where $K_1$ and $K_2$ are matrices in $SO(4)$ and $F$ is a matrix of the form

$$
F = e^L.
$$

(16)
Here $L$ is a matrix in a (three dimensional) maximal Abelian subalgebra $A$ in $S$. Moreover $A$ can be chosen to be spanned by the matrix $A$ in (8) and $A_1 := \text{diag}(-i, 3i, -i, -i)$ and $A_2 := \text{diag}(-i, -i, 3i, -i)$. Using the fact that $A_1$ and $A_2$ are similar to $A$ via a similarity transformation in $SO(4)$ and that $A$ is Abelian, we can write every element $F = e^L$, with $L \in A$, as

$$F = K_4 e^{A_3}K_3 e^{A_2}K_2 e^{A_1}K_1,$$

with $K_j \in SO(4), j = 1, 2, 3, 4; t_1, t_2, t_3$ can be chosen nonnegative since the subgroup $\{ P \in SU(4) | P = e^{A_s}, s \in R \}$ is closed. Comparing (17) with (15), we obtain (14). \hfill \Box

An alternative to the Cartan decomposition (14) is described in [7]. The decomposition in [7] leads to a higher number of factors but has the merit to be amenable of a simple analytic procedure [23] to determine the factors. On the other hand, there is no general analytic procedure to determine the factors in (14). One can express each of the factors in $SO(4)$ using the parametrizations of the Lie group $SO(4)$ given in [4], [23] and then determine the parameters by numerically solving a set of nonlinear algebraic equations. In this context, in order to keep the number of variables low, it is convenient to work with equation (15) rather than (14). We will keep referring to the decomposition (14) although everything we will say can be adapted with minimum changes to the decomposition discussed in [7].

Given a decomposition such as (14) the strategy of control advocated in [6], [18] consists of steering to each one of the factors separately. The steering to an element of the form $e^{A_t}$ can be obtained by setting the control equal to zero for time $t$. The steering to elements in $SO(4)$ can be obtained with very high amplitude, short time, controls designed to steer the state of system (13) and that essentially render the effect of the drift term $AX$ negligible. In practice, one has constraints on the magnitude of the control which will give a non zero error. This error will be small for small transfer time as described in the following theorem.

**Theorem 2.2** Let $K_j \in SO(4)$ denote a desired final condition for system (7) and let $u_j(t)$ be a control function steering the state of (13) to $K_j$ in time $T$. Then, if $X_1(t)$ denotes the trajectory of system (7) with the same control, we have, for some constants $M$ and $N$ independent of $u_j$, 1

$$||X_1(T) - K_j|| < NT + MN ||u_j||_{\infty} T^2 e^{M||u_j||_{\infty} T}$$

**Proof.** Define

$$F_j(t) := B_x u_{jx}(t) + B_y u_{jy}(t) + B_z u_{jz}(t),$$

where $u_{jx}$, $u_{jy}$ and $u_{jz}$ are the $x, y$ and $z$ components of the control function $u_j$. Call $X_1(t)$ and $X_2(t)$ the trajectories corresponding to the system in (7) and (13) respectively with this

\footnote{We denote by $||u_j||_{\infty} := \max_{t \in [0, T]} \sqrt{u_{jx}^2(t) + u_{jy}^2(t) + u_{jz}^2(t)}$, where $u_{jx, y, z}$ are the $x, y, z$ components of $u_j$.}
control. We have
\[ X_1(t) = I + \int_0^t F_j(s)X_1(s)ds + \int_0^t AX_1(s)ds, \tag{20} \]
and
\[ X_2(t) = I + \int_0^t F_j(s)X_2(s)ds. \tag{21} \]
By subtracting (21) from (20), we obtain
\[ ||X_1(t) - X_2(t)|| \leq \int_0^t ||F_j(s)|| ||X_1(s) - X_2(s)|| ds + \int_0^t ||A|| ||X_1(s)|| ds. \tag{22} \]
Now define \( M := ||B_x|| + ||B_y|| + ||B_z|| \) and, using compactness of \( SU(4) \), choose a constant \( N \) such that
\[ ||A|| ||X|| \leq N, \tag{23} \]
for every \( X \in SU(4) \). Using these definitions in (22), we obtain
\[ ||X_1(t) - X_2(t)|| \leq M||u||_\infty \int_0^t ||X_1(s) - X_2(s)|| ds + Nt. \tag{24} \]
Using Gronwall-Bellmann inequality, we obtain
\[ ||X_1(t) - X_2(t)|| \leq Nt + MN||u||_\infty \int_0^t s e^{M||u||_\infty (t-s)} ds < Nt + MN||u||_\infty \frac{T^2}{2} e^{M||u||_\infty}. \tag{25} \]
Setting \( t = T \) in (25), we obtain (18).

Given a value for the maximum of the norm of the control, \( ||u||_\infty \) and a time of transfer \( T \), Theorem 2.2 provides a bound on the error that one has by neglecting the drift term and applying the same control as for system (13) to system (7). Since we would like to minimize this bound, given a physical limit \( \gamma \) on the magnitude of the control, we would like to find \( u_j \) steering the state of (13) to \( K_j \) and minimizing the right hand side of (18). The control solving this problem is the same control which steers the state of (13) to \( K_j \) in minimum time, \( T_{min} \), subject to \( ||.||_\infty \leq \gamma \). To see this, let us call \( \tilde{u}_j \) the control steering to \( K_j \) and minimizing
\[ J(T, ||u||_\infty) := NT + MN||u||_\infty \frac{T^2}{2} e^{M||u||_\infty}. \tag{26} \]
Let \( \tilde{T} \), with \( \tilde{T} > T_{min} \) be the time required for the state transfer with the control \( \tilde{u}_j \). It cannot be \( ||\tilde{u}_j||_\infty = \gamma \) because the time minimizing control (which also has \( ||.||_\infty \leq \gamma \)) would lead to a smaller cost \( J(T, ||u||_\infty) \) in (26). If \( ||\tilde{u}_j||_\infty < \gamma \), the control \( \frac{\gamma}{||\tilde{u}_j||_\infty} \tilde{u}_j (\frac{\gamma}{||\tilde{u}_j||_\infty} t) \), which has norm \( ||.||_\infty \) equal to \( \gamma \), steers the state of (13) to \( K_j \) in time \( \frac{||\tilde{u}_j||_\infty}{\gamma} \tilde{T} \) and gives for the cost (26) the value
\[ J = N \frac{||\tilde{u}_j||_\infty}{\gamma} \tilde{T} + \frac{||\tilde{u}_j||_\infty}{\gamma} MN||u||_\infty \frac{\tilde{T}^2}{2} e^{M||u||_\infty} < N\tilde{T} + MN||u||_\infty \frac{\tilde{T}^2}{2} e^{M||u||_\infty} \tag{27} \]
Motivated by this analysis, we shall treat in the following sections the time optimal control problem on \( SO(4) \).
3 Formulation of the Optimal Control Problem on \( SO(4) \)

Consider the system

\[
\dot{X} = B_x X u_x + B_y X u_y + B_z X u_z,
\]

with initial condition equal to the identity \( I_{4 \times 4} \). The functions \( u_x, u_y, \) and \( u_z \) are required to be Lebesgue measurable in the interval where they are defined \([0, T]\) and they are such that

\[
u_x^2(t) + u_y^2(t) + u_z^2(t) \leq \gamma^2,
\]

for every \( t \in [0, T] \), and a prescribed \( \gamma > 0 \). Given a desired final condition \( X_f \) for the state \( X \) in (28), the problem is to find a set of functions \( u_x, u_y, u_z \), defined in \([0, T]\) such that the corresponding solution of (28), \( X \), satisfies \( X(T) = X_f \), and \( T \) is minimum. Notice that (see e.g. [2], [4]), since \( B_x, B_y, B_z \) in (9), (10), (11) generate the whole Lie algebra \( so(4) \), without bound on the control functions, every state could be reached in arbitrary small time. Therefore, the bound in (29) is necessary for the minimum time problem to be well posed. Moreover, it follows from a result in [17] that the given system is controllable with arbitrarily bounded controls, namely, for every value of \( \gamma \) in (29), and for every desired final condition \( X_f \) in \( SO(4) \), there exists a set of control functions, \( u_x, u_y, u_z \), driving the state to \( X_f \). We can combine this result with existence theorems for optimal control problems (see e.g. Theorem III.4.1 in [12]) to conclude that the optimal control problem just stated has a solution\(^2\) The optimal minimum time control therefore exists and can be found among the ones that satisfy the Pontryagin necessary conditions. These conditions are given in the following theorem [1] [12] [28].

**Theorem 3.1.** Assume that \( u_x^0, u_y^0, u_z^0 \), is the optimal Lebesgue measurable control steering the state of the system (28) from the identity to a final target state \( X_f \) in minimum time \( T \), satisfying the constraint (29). Denote by \( X_0 \) the corresponding trajectory for \( X \). Then, there exists a matrix \( M \in so(4) \) and a constant \( \lambda \leq 0 \) such that almost everywhere\(^3\)

\[
\langle M, X^*_0(t) B_x X_0(t) \rangle u_x^0(t) + \langle M, X^*_0(t) B_y X_0(t) \rangle u_y^0(t) + \langle M, X^*_0(t) B_z X_0(t) \rangle u_z^0(t) = \
\min_{v_x,v_y,v_z} \langle M, X^*_0(t) B_x X_0(t) \rangle v_x + \langle M, X^*_0(t) B_y X_0(t) \rangle v_y + \langle M, X^*_0(t) B_z X_0(t) \rangle v_z = \lambda,
\]

where the minimum is taken over all the triples \( v_x, v_y, v_z \) which satisfy \( v_x^2 + v_y^2 + v_z^2 \leq \gamma^2 \). The matrix \( M \) and the constant \( \lambda \) cannot be both zero.

\(^2\)The same considerations hold if one considers a steering problem with minimum energy, where the cost functional has the form

\[
\int_0^T \sum_{j,k} q_{jk} u_j u_k,
\]

with \( q_{jk} \) a positive definite form.

\(^3\)The inner product \( \langle A, B \rangle \) between two matrices in \( su(4) \) is defined as \( \langle A, B \rangle := \text{Trace}(A, B^*) \), where \( * \) denotes transposed conjugate.
In the above theorem, if \( \lambda = 0 \) then the minimization condition implies that almost everywhere
\[
\langle M, X_0^*(t)B_{x,y,z}X_0(t) \rangle = 0.
\] (31)
Controls that satisfy (30) with \( \lambda = 0 \) are called \textit{abnormal extremals}. The condition \( \lambda \neq 0 \) means that, almost everywhere, at least one among \( \langle MX_0^*(t)B_{x,y,z}X_0(t) \rangle \) is different from zero. Controls that satisfy (30) with \( \lambda \neq 0 \) are called \textit{normal extremals}. Characterization of normal and abnormal extremals is given in the next section.

4 Characterization of Abnormal and Normal Extremals

We will use, in the sequel, the following definitions
\[
C_x := [B_y, B_z], \quad C_y := [B_z, B_x], \quad C_z := [B_x, B_y],
\] (32)
The subspaces
\[
A_x := \text{span}\{B_x, C_x\}, \quad A_y := \text{span}\{B_y, C_y\}, \quad A_z := \text{span}\{B_z, C_z\},
\] (33)
are the three Abelian subalgebras of \( so(4) \) whose direct sum gives \( so(4) \), and
\[
\] (34)

In the following Theorem, we characterize the abnormal extremals.

\textbf{Theorem 4.1} Every abnormal extremal has the form
\[
u_x(t) := c_1\phi(t), \quad u_y(t) := c_2\phi(t), \quad u_z(t) := c_3\phi(t),
\] (35)
for some constants \( c_1, c_2, c_3 \) and a function \( \phi(t) \) with
\[
\phi^2(t) \leq \frac{\gamma^2}{c_1^2 + c_2^2 + c_3^2},
\] (36)
for every \( t \) in its domain [0, T].

\textbf{Proof.} Assume that \( \lambda = 0 \) in (30), then the minimization condition implies almost everywhere, and, by continuity, everywhere, in the interval where the extremal control is defined, [0, T],
\[
\langle M, X_0^*(t)B_zX_0(t) \rangle \equiv 0,
\] (37)
\[
\langle M, X_0^*(t)B_yX_0(t) \rangle \equiv 0,
\] (38)
\[
\langle M, X_0^*(t)B_xX_0(t) \rangle \equiv 0.
\] (39)
By differentiating (37), (38) and (39), taking into account (28) and (32), we obtain a.e.

$$\langle M, X_0^*(t)C_x X_0(t)\rangle u_y(t) - \langle M, X_0^*(t)C_y X_0(t)\rangle u_z(t) = 0,$$

\hspace{1cm} (40)

$$\langle M, X_0^*(t)C_x X_0(t)\rangle u_z(t) - \langle M, X_0^*(t)C_x X_0(t)\rangle u_x(t) = 0,$$

\hspace{1cm} (41)

$$\langle M, X_0^*(t)C_y X_0(t)\rangle u_x(t) - \langle M, X_0^*(t)C_x X_0(t)\rangle u_y(t) = 0.$$  \hspace{1cm} (42)

By differentiating with respect to time \(\langle M, X_0(t)C_x X_0(t)\rangle\), we obtain, using the fact that \(B_x\) and \(C_x\) commute,

$$\frac{d}{dt} \langle M, X_0^*(t)C_x X_0(t)\rangle = \langle M, X_0^*(t)[C_x, B_y]X_0(t)\rangle u_y(t) + \langle M, X_0^*(t)[C_x, B_z]X_0(t)\rangle u_z(t),$$

\hspace{1cm} (43)

almost everywhere. From (34), we know that \([C_x, B_y] \in \mathcal{A}_z\) and \([C_x, B_z] \in \mathcal{A}_y\). A direct calculation shows

$$[C_x, B_y] = -4r B_z - 2(r + 1) C_z,$$

\hspace{1cm} (44)

and

$$[C_x, B_z] = 2(r + 1) C_y + 4r B_y.$$  \hspace{1cm} (45)

Replacing this into (43), we obtain a.e.

$$\frac{d}{dt} \langle M, X_0^*(t)C_x X_0(t)\rangle =$$

\hspace{1cm} 

$$-4r\langle M, X_0^*(t)B_z X_0(t)\rangle u_y(t) + 4r\langle M, X_0^*(t)B_y X_0(t)\rangle u_z(t) +$$

\hspace{1cm} 

$$2(r + 1)(\langle M, X_0^*(t)C_y X_0(t)\rangle u_z(t) - 2(r + 1)\langle M, X_0^*(t)C_x X_0(t)\rangle u_y(t)),$$

\hspace{1cm} (46)

and, using (40) along with (38) and (39), we obtain a.e. \(\frac{d}{dt} \langle M, X_0^*(t)C_x X_0(t)\rangle = 0\), and by absolute continuity,

$$\langle M, X_0^*(t)C_x X_0(t)\rangle \equiv constant := k_1.$$  \hspace{1cm} (47)

A similar argument gives

$$\langle M, X_0^*(t)C_y X_0(t)\rangle \equiv constant := k_2,$$

\hspace{1cm} (48)

and

$$\langle M, X_0^*(t)C_z X_0(t)\rangle \equiv constant := k_3.$$  \hspace{1cm} (49)

Now, replacing (47), (48) and (49) into (40), (41), (42), we obtain (a.e.)

$$k_3 u_y(t) - k_2 u_z(t) = 0,$$

\hspace{1cm} (50)

$$k_1 u_z(t) - k_3 u_x(t) = 0,$$

\hspace{1cm} 

$$k_2 u_x(t) - k_1 u_y(t) = 0.$$
$c_3 \phi(t)$, for some measurable function $\phi(t)$ and $[c_1, c_2, c_3]^T$ in the kernel of the matrix of coefficients in (50). The condition (36) follows from the bound (29).

The following Theorem gives a characterization of the normal extremals.

**Theorem 4.2.** Every normal extremals $\vec{u} := [u_x, u_y, u_z]^T$ is a solution of a linear system

$$\dot{\vec{u}} = F\vec{u},$$

where $F$ is a $3 \times 3$ skew-symmetric matrix.

**Proof.** If $\lambda \neq 0$ in (30), then, at a given time, at least one among $\langle M, X_0^*B_xX_0 \rangle$, $\langle M, X_0^*B_yX_0 \rangle$ and $\langle M, X_0^*B_zX_0 \rangle$ is different from zero. The minimization condition gives that, for a suitable $M \in \text{so}(4)$,

$$u_x = -\langle M, X_0^*B_xX_0 \rangle,$$

$$u_y = -\langle M, X_0^*B_yX_0 \rangle,$$

$$u_z = -\langle M, X_0^*B_zX_0 \rangle.$$  

Also, define

$$a_x = -\langle M, X_0^*C_xX_0 \rangle,$$

$$a_y = -\langle M, X_0^*C_yX_0 \rangle,$$

$$a_z = -\langle M, X_0^*C_zX_0 \rangle,$$

with $C_x$, $C_y$ and $C_z$ defined in (32). By differentiating (52), (53), (54), we obtain (cfr. the proof of Theorem 4.1)

$$\dot{a}_x = a_zu_y - a_yu_z,$$

$$\dot{a}_y = a_xu_z - a_zu_x,$$

$$\dot{a}_z = a_yu_x - a_xu_y.$$  

Also, by differentiating (55) and recalling (44) and (45), we obtain,

$$\dot{a}_x = 2(r + 1)(a_zu_y - a_yu_z).$$

Analogously, by differentiating (56) and (57), we obtain

$$\dot{a}_y = 2(r + 1)(a_xu_z - a_zu_x),$$

$$\dot{a}_z = 2(r + 1)(a_yu_x - a_xu_y).$$

\footnote{We omit the ‘(a.e.)’ in the following for brevity. All of the equations hold (a.e.), however (51) holds everywhere.}
Comparison of (61), (62), (63) with (58), (59), (60) gives

\[ \begin{align*}
\dot{a}_x &= 2(r+1)\dot{a}_x, \\
\dot{a}_y &= 2(r+1)\dot{a}_y, \\
\dot{a}_z &= 2(r+1)\dot{a}_z.
\end{align*} \] (64)-(66)

Integrating these equations and substituting into (58), (59), (60), we obtain

\[ \begin{align*}
\dot{u}_x &= [a_x(0) - 2(r+1)u_x(0)]u_y - [a_y(0) - 2(r+1)u_y(0)]u_z, \\
\dot{u}_y &= [a_x(0) - 2(r+1)u_x(0)]u_z - [a_z(0) - 2(r+1)u_z(0)]u_x, \\
\dot{u}_z &= [a_y(0) - 2(r+1)u_y(0)]u_x - [a_x(0) - 2(r+1)u_x(0)]u_y.
\end{align*} \] (67)-(69)

### 5 Discussion

Assume a desired final state for system (28) is given. As for abnormal extremals, notice that the matrix \( M \in \text{so}(4) \), in the statement of the maximum principle in Theorem 3.1, has to be orthogonal to \( B_x, B_y \) and \( B_z \) (see (41)-(43)). Using the fact that the subspaces \( A_x, A_y \) and \( A_z \), defined in (33) are orthogonal to each other, it can be easily seen that \( M \) has the form \( M = aD_x + bD_y + cD_z \), where \( D_{x,y,z} \in A_{x,y,z} \) is perpendicular to \( B_{x,y,z} \). The matrix \( X_f \) has to be of the form

\[ X_f := e^{c_1B_x+c_2B_y+c_3B_z}, \] (70)

for some constants \( c_1, c_2, c_3 \). Notice that because of the bound (29), for every extremal of the form

\[ u_x := c_1\phi(t), \quad u_y(t) := c_2\phi(t), \quad u_z := c_3\phi(t), \] (71)

one can consider a constant control giving a state transfer to the same final condition in (possibly) less time, so that there is no loss in considering only constant controls. As an example of an abnormal extremal, consider the final condition \( X_f = e^{B_z} \). The control \( u_x(t) \equiv \gamma, u_y(t) \equiv 0, u_z(t) \equiv 0 \) is an abnormal extremal. The matrix \( M \) can be chosen in \( A_x \), perpendicular to \( B_x \). Conditions (37), (38), (39) are verified with \( X(t) = e^{\gamma B_z t} \), for every \( t \in [0, \frac{1}{7}] \) because \( M \) is perpendicular to \( B_x, B_y \) and \( B_z \) and it commutes with \( B_z \).

Theorem 4.2 proves that normal extremals are solutions of a linear system of equations (51) where the matrix of coefficients is skew-symmetric. In general the solution will depend on 6 parameters: The three constants \( k_1 := [a_x(0) - 2(r+1)u_x(0)], k_2 := [a_y(0) - 2(r+1)u_y(0)], k_3 := [a_z(0) - 2(r+1)u_z(0)] \) and the initial conditions \( u_x(0), u_y(0) \) and \( u_z(0) \). These parameters depend linearly on the six entries of the matrix \( M \) through (52)-(57). They have to be tuned so that the corresponding trajectory \( X = X(t) \) obtains \( X(T) = X_f \), in minimum time \( T \). The tuning of the parameters can be simplified by the following considerations: From (64)-(66), we have that at every time \( t \)

\[ a_{x,y,z}(t) - a_{x,y,z}(0) = 2(r+1)(u_{x,y,z}(t) - u_{x,y,z}(0)). \] (72)
Writing this for the final time and substituting the desired final condition $X_f$ in the definitions (52)-(57), we obtain three linear algebraic equations in the parameters of the matrix $M$ that can be used to decrease the number of parameters of up to three. Moreover $u_x^2(t) + u_y^2(t) + u_z^2(t)$ is constant at every time $t$ and it can be chosen to be equal to $\gamma^2$ since every value $< \gamma^2$ would not lead to a time optimal control law (cfr. discussion at the end of Section 2). Therefore, given $P_0 := [u_x(0), u_y(0), u_z(0)]^T$ on the three dimensional sphere of radius $\gamma$ and considered the coefficients $k_1$, $k_2$, $k_3$ of the matrix $F$ in (51), the evolution in (51) will carry $P_0$ into another point on the same sphere through a rotation. More precisely, at every time $t$, $[u_x(t), u_y(t), u_z(t)]^T$ will be on the sphere of radius $\gamma$ and on a plane perpendicular to the axis of rotation, which is given by $[k_1, k_2, k_3]^T$, and containing $P_0$. Therefore we have for every $t$

$$k_1(u_x(t) - u_x(0)) + k_2(u_y(t) - u_y(0)) + k_3(u_z(t) - u_z(0)) = 0,$$

(73)

$$u_x^2(t) + u_y^2(t) + u_z^2(t) = \gamma^2.$$  

(74)

Writing these two equations for the final time and replacing the final condition into (52)-(54), we obtain two algebraic equations to be solved in terms of the free parameters. To each solution there corresponds a control to be tested in equation (28).

6 Concluding Remarks

The new application of computing requires the development of methods to drive the state of quantum systems with high accuracy. In this paper, an algorithm for the control of a coupled spin $\frac{1}{2}$ particles system has been derived which yields a final configuration as close to the target as desired. In the spirit of [6], [18], this algorithms uses a Lie group decomposition of $SU(4)$ and a control algorithm on the Lie group $SO(4)$. The price for an increase in accuracy is an increase of the magnitude of the control. Therefore, we asked the question of what control is the best, given a constraint on the magnitude. This lead to a treatment of the time optimal control problem on $SO(4)$. We showed that explicit expressions for the time optimal control functions can be obtained. These are solutions of a linear system of differential equations with skew-symmetric coefficient matrix.

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References


