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SPACE-TIME EVOLUTION OF WAVE FUNCTIONS; CONTROL OF QUANTUM DYNAMICS WITH THE HELP OF COHERENT PROCESSES

Time-Optimal Torus Theorem and Control of Spin Systems[1]

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Abstract—Given a compact, connected Lie group G with Lie algebra $\mathfrak{g}$. We discuss time-optimal control of bilinear systems of the form

$$\dot{U}(t) = \left(H_d + \sum_{j=1}^{m} v_j(t) H_j\right) U(t), \tag{I}$$

where $H_d, H_j \in \mathfrak{g}$, $U \in G$, and the v_j act as control variables. The case $G = SU(2^n)$ has found interesting applications to questions of time-optimal control of spin systems. In this context Eq. (I) describes the dynamics of an n-particle system with fixed drift Hamiltonian H_d, which is to be controlled by a number of exterior magnetic fields of variable strength, proportional to the parameters v_j. The question of interest here is to transfer the system from a given initial state U_0 to a prescribed final state U_1 in least possible time. Denote by $\mathfrak{k}$ the Lie algebra spanned by $H_1, \ldots, H_m$, and by K the corresponding Lie subgroup of G. After reformulating the optimal control problem for system (I) in terms of an equivalent problem on the homogeneous space G/K we discuss in detail time-optimal control strategies for system (I) in the case where G/K carries the structure of a Riemannian symmetric space.

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1. INTRODUCTION

Given the Lie group $G = SU(2^n)$, together with a fixed set of skew Hermitian operators,

$$H_d, H_1, \ldots, H_m: \quad (\mathbb{C}^2)^{\otimes n} \longrightarrow (\mathbb{C}^2)^{\otimes n}.$$

They define the following family of skew Hermitian operators:

$$H(v_1, \ldots, v_m) = H_d + \sum_{j=1}^{m} v_j H_j,$$

$$v = (v_1, \ldots, v_m) \in \mathbb{R}^m.$$

Fix an element $U_F \in G$ and consider the right-invariant control system on G given by

$$\dot{U} = -\mathrm{i}H(v)U, \quad U(0) = \mathbf{1} \tag{1}$$

with v acting as the control variable. The question of interest to us is whether it is possible to steer system (1) from the initial state $U(0) = \mathbf{1}$ to the final state U_F. If this is the case, what will be the minimum amount of time to achieve such a transfer? The motivation for treating that kind of problem in time-optimal control theory arises from questions concerning the quantum mechanics of spin systems such as ensembles of electrons or neutrons. Indeed, the operator $H(v)$ plays the role of a time-dependent Hamiltonian for a system of coupled spin particles that are under the influence of an exterior magnetic field of fixed direction and variable strength (modelled by the variable v). So (1) is just Schrödinger's equation for the time-evolution operator U of such a system (with Planck's constant $\hbar$ set equal to 1).

The desire to solve a control problem as formulated above came alongside with the development of certain experiments in nuclear magnetic resonance spectroscopy (NMR) and quantum computing. Here one needs to manipulate ensembles of coupled nuclear spins and wishes to do so in least possible time. See, e.g., [1, 2] for details on this topic. In the discussion to follow we are going to generalize this kind of control problem from the specific case $G = SU(2^n)$ to arbitrary compact, connected Lie groups.

2. EQUIVALENCE THEOREM

Throughout this section G denotes a compact Lie group with Lie algebra $\mathfrak{g}$, while K denotes a closed sub-

[1] The text was submitted by the author in English.

group of G with Lie algebra $\mathfrak{k}$. Note that the assumption on K to be closed in G guarantees that the space of left cosets,

$$G/K = \{gK|g \in G\},$$

is also a smooth manifold (of dimension $\dim(G/K) = \dim(G) - \dim(K)$) such that the canonical projection π: $g \mapsto gK = [g]$ is smooth. It carries a natural transitive action of G, which is given by

$$hgK := (hg)K$$

and thus will be called a homogeneous space for the group G. We are interested in the following affine right-invariant control system on the Lie group G:

$$\dot{U} = \left(H_d + \sum_{j=1}^{m} v_j H_j\right)U, \quad U(0) = \mathbf{1}, \qquad (2)$$

with $H_d \in \mathfrak{g}$ arbitrary but fixed and $H_1, \ldots, H_m$ a fixed set of generators for the Lie algebra $\mathfrak{k}$.

Definition 2.1. The control system (2) will from now on be referred to as the unreduced system. We furthermore define on G the adjoint system to be

$$\dot{U} = XU, \quad U(0) = \mathbf{1}, \quad X \in \mathrm{Ad}_K H_d. \qquad (3)$$

Here, $\mathrm{Ad}_K H_d$ denotes the adjoint orbit of $H_d \in \mathfrak{g}$ under K, which is

$$\mathrm{Ad}_K H_d = \{kH_d k^{-1}|k \in K\} \subseteq \mathfrak{g}.$$

On the homogeneous space G/K, let us define the reduced system to be

$$\dot{P} = XP, \quad P(0) = [\mathbf{1}], \quad X \in \mathrm{Ad}_K H_d, \qquad (4)$$

where the expression XP is explained as follows. Let R_g: $G \longrightarrow G$ be the right-translation by $g \in G$, $R_g(h) := hg$. If $P = \pi(g) = [g] \in G/K$, then let

$$XP := D_1(\pi \circ R_g)(X) \in T_g(G/K). \qquad (5)$$

Before proceeding in our discussion of time-optimal control of spin systems, it will be convenient to introduce some general notions from control theory.

Definition 2.2. Let Σ be a control system on the manifold M with admissible vector fields $f_u \in \mathrm{Vect}(M)$, where u is contained in a fixed set $U \subseteq \mathbb{R}^m$ of control parameters. Fix $x_0 \in M$ and let $T \geq 0$. We define $R(x_0, T)$ to be the set of all $x_F \in M$ with the property that there exists a control function u: $[0, T] \longrightarrow U$ which generates a trajectory $t \mapsto x(t)$ such that $x(0) = x_0$ and $x(T) = x_F$ (i.e., we have that $\dot{x}(t) = f_{u(t)}$ holds almost everywhere on $[0, T]$). This set $R(x_0, T)$ is called the set of reachable points from x_0 at time T.

Define furthermore the reachable set from x_0 within time T to be

$$\mathbf{R}(x_0, T) = \bigcup_{0 \leq t \leq T} R(x_0, t) \qquad (6)$$

and the reachable set for x_0 to be

$$\mathbf{R}(x_0) = \bigcup_{0 \leq T < \infty} \mathbf{R}(x_0, T). \qquad (7)$$

The system Σ is called controllable if $\mathbf{R}(x_0) = M$ holds.

We next define the set $S(x, t_0)$ of approximately reachable points from x_0 within time $t_0 \geq 0$ to be

$$S(x_0, t_0) := \bigcap_{t > t_0} \overline{\mathbf{R}(x, t)}. \qquad (8)$$

Thus a point $y \in M$ is contained in $S(x_0, t_0)$ if and only if for any neighbourhood W of y and any $\varepsilon > 0$ there exists a point $z \in W \cap \mathbf{R}(x_0, t_0 + \varepsilon)$. We finally define the infimizing time to steer Σ from x_0 to $x_1 \in M$ to be

$$t_{\mathrm{int}}(x_0, x_1) := \inf\{t \in \mathbb{R}|x_1 \in S(x_0, t)\}.$$

With those definitions at hand, we are able to make a precise statement on the relation between the control systems (2)–(4) as introduced before.

Theorem 2.3. (Equivalence theorem). *Label the reachable and approximately reachable sets for the unreduced, adjoint, and reduced systems of Definition* 2.1 *by lower case indices* 1, 2, *and* 3, *respectively. Then for all* $t \geq 0$ *the following holds*:

$$\text{(i)} \quad S_1(\mathbf{1}, t) = K\overline{R_2(\mathbf{1}, t)} = \overline{R_2(\mathbf{1}, t)}K,$$

$$\text{(ii)} \quad \pi(S_1(\mathbf{1}, t)) = \overline{R_3([\mathbf{1}], t)}.$$

Proof. (see [3]). The previous theorem enables us to reduce the study of the original unreduced system (2) on the Lie group G to the reduced system (4) on the homogenous space G/K. Namely, not only the approximately reachable set $S_1(1, t)$ of system (2) is determined (modulo K) by the strictly reachable set $R_3([\mathbf{1}], t)$ of (4), but it is even possible to construct optimal control strategies for system (2) from those of system (4), cf., the discussion at the end of Section 3.

From a control theoretic perspective, it is favorable to consider system (4) rather than system (2) for the following reasons. Firstly, the set of control variables $\mathrm{Ad}_K H_d$ in the reduced case is, in contrast to the unreduced case, compact. Thus it is no longer possible to steer in any direction at an arbitrarily high speed so that the distinction between approximately and strictly reachable sets becomes superfluous. Secondly, the compactness makes it possible to apply standard methods from optimal control theory, such as Pontrjagin's maximum principle (cf. [4, 5]), to obtain extremal trajectories. Finally, the proof of the time-optimal torus theorem as formulated in Section 3 relies on the equivalent description of the original system (2) through Theorem 2.3, and in particular on the invariance of the set $\mathrm{Ad}_K H_d$ of control variables under conjugation by elements of K.

3. TIME-OPTIMAL TORUS THEOREM

In this section we shall specialize our discussion to the case of homogeneous spaces G/K, which meet the additional symmetry condition as introduced in the following definition.

Definition 3.1. Let $\mathfrak{k}$ be a Lie subalgebra of $\mathfrak{g}$. The pair $(\mathfrak{g}, \mathfrak{k})$ is called a symmetric Lie algebra pair if there exists a vector space $\mathfrak{p} \subseteq \mathfrak{g}$ such that

$$\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p},$$

$$[\mathfrak{p}, \mathfrak{p}] \subseteq \mathfrak{k}, \quad [\mathfrak{k}, \mathfrak{p}] \subseteq \mathfrak{p}.$$

The direct sum decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ is then named Cartan-like decomposition of $\mathfrak{g}$. A homogeneous space G/K is called symmetric if the corresponding Lie algebra pair $(\mathfrak{g}, \mathfrak{k})$ is symmetric.

There is a very well developed theory of symmetric spaces (cf. [6]). To us the following features are the most relevant.

For any two maximal abelian subalgebras $\mathfrak{h}, \mathfrak{h}' \subseteq \mathfrak{p}$ (i.e., $[\mathfrak{h}, \mathfrak{h}] = 0$ and $\mathfrak{h}$ is not contained in any bigger abelian subalgebra of $\mathfrak{g}$ in $\mathfrak{p}$, and the same holds for $\mathfrak{h}'$), there exists $k \in K$ such that $\mathfrak{h}' = \mathrm{Ad}_k\mathfrak{h}$.

The corresponding tori $A, A' \subseteq G$ with Lie algebras $\mathfrak{h}, \mathfrak{h}'$ are conjugate by the same k, i.e., $A' = kAk^{-1}$.

Any $[p] \in G/K$ is of the form $[p] = [ktk^{-1}]$ for suitable $t \in A$ and $k \in K$.

For each $X \in \mathfrak{h}$ we have that

$$\mathbb{O}(X) := \mathrm{Ad}_K X \cap \mathfrak{h}$$

is a finite subset of $\mathfrak{h}$. It is called the Weyl orbit of X under K. Its convex hull $\mathcal{C}\mathbb{O}(X)$ equals the image of $\mathrm{Ad}_K X$ under orthogonal projection onto $\mathfrak{h}$.

In the following an explicit solution to the control problem as described in Section 1 and reformulated as Equivalence Theorem 2.3 will be discussed under the additional assumption that the homogeneous space G/K in Theorem 2.3 gives rise to a symmetric Lie algebra pair $(\mathfrak{g}, \mathfrak{k})$. Thus in the following we fix a compact Lie group G together with a closed subgroup K such that the coset space G/K is symmetric in the sense of Definition 3.1. For simplicity we further assume G to be simply connected and semisimple (i.e., the Killing form $\kappa(X, Y) = \mathrm{tr}(XY)$ defines a nondegenerate bilinear form on $\mathfrak{g}$). Let $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}$ be the corresponding Cartan-like decomposition, and take $\mathfrak{h} \subseteq \mathfrak{p}$ to be a maximal abelian subalgebra of $\mathfrak{p}$. Denote by A the torus in G with Lie algebra $\mathfrak{h}$.

Theorem 3.2. (Controllability). *On the symmetric space G/K, consider the reduced system* (4). *Assume that the projection H_0 of H_d on $\mathfrak{p}$ is contained in the subalgebra $\mathfrak{h} \subseteq \mathfrak{p}$, but does not lie in any root hyperplane of the root space decomposition of $\mathfrak{g}_{\mathbb{C}}$ with respect to $\mathfrak{h}$ (cf.* [6]*). Then system* (6) *has reachable set* $\mathbf{R}([\mathbf{1}]) = G/K$*, i.e., it is controllable.*

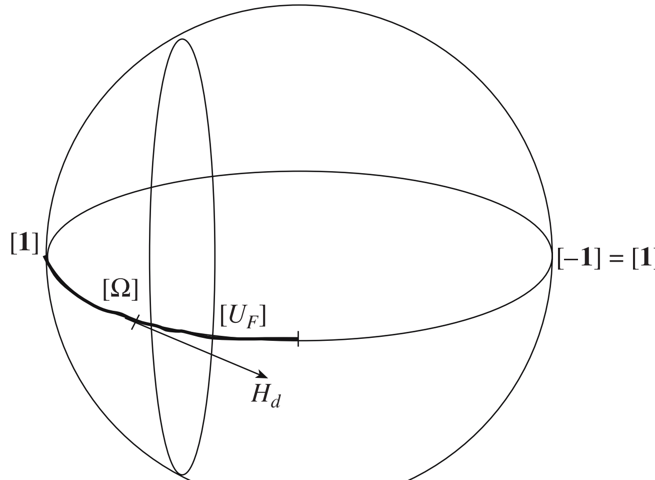

Fig. 1. Time-optimal control of a single-particle spin system. The underlying manifold for the reduced system is $G/K = \mathbb{RP}^2$. Terminal points lying on circles perpendicularly to the equator can be considered equivalent and thus be replaced by a point $[U_F] \in [\Omega]$. Time-optimal trajectories between $[\mathbf{1}]$ and $[U_F]$ may always be chosen to be contained in $[\Omega]$ and are then generated by the elements $\mathbb{O}(H_d) = \pm H_d$ in the Weyl orbit of H_d.

Proof. One first proves the result for the unreduced system (2). Here the root-space decomposition of $\mathfrak{g}_{\mathbb{C}}$ with respect to a maximal abelian subalgebra $\mathfrak{t}$ of $\mathfrak{g}$, where $\mathfrak{h} \subseteq \mathfrak{t}$, is used to show that the Lie algebra generated by $\mathfrak{k}$ and H_d is equal to $\mathfrak{g}$. This is sufficient for controllability of system (2), cf. [4]. The statement on the controllability of the reduced system is then an immediate consequence of Theorem 2.3 (ii). For details see [3].

Remark 3.3. A different proof of Theorem 3.2, without the assumption that H_0 is not contained in any root hyperplane, can be found in [7].

We now turn to a discussion of time-optimal control and start with heuristic considerations for the case $n = 1$ of a single particle system. Here the underlying manifold G/K for the reduced control system

$$\dot{P} = XP, \quad P(0) = [\mathbf{1}], \quad X \in \mathrm{Ad}_K H_d$$

is $G/K = SU(2)/SU(1)$ and thus diffeomorphic to the real projective space $\mathbb{RP}^2$ one obtains after identifying antipodal points in the 2-sphere $\mathbb{S}^2$, cf., Fig. 1.

The drift Hamiltonian we want to consider is

$$H_d = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \in \mathfrak{su}(2).$$

The subgroup K of G generated by the control Hamiltonian is chosen to be

$$K = \left\{ \begin{pmatrix} \cos(\phi) & \sin(\phi) \\ -\sin(\phi) & \cos(\phi) \end{pmatrix} \middle| \phi \in \mathbb{R} \right\}.$$

Then the set $\mathrm{Ad}_K H_d$ can be described as

$$\mathrm{Ad}_K H_d = \left\{ i\begin{pmatrix} \alpha & \beta \\ \beta & -\alpha \end{pmatrix} \middle| \alpha, \beta \in \mathbb{R} \right\},$$

i.e., the subset of symmetric matrices in $\mathfrak{g} = \mathfrak{su}(2)$. This set also can be identified with the unit sphere of the tangent space $T_{[\mathbf{1}]}G/H$ of G/H at [**1**]. So we are here in the special situation that the reduced system can be steered (at unit speed) in any possible direction of G/H. This is no longer true in higher dimensional symmetric spaces.

Now let $[U_F] \in G/K$ be an arbitrary terminal state. The first observation is that one can replace $[U_F]$ by any other point

$$[kU_Fk^{-1}] = [kU_F] \in G/K, \quad k \in K$$

without essentially changing the control problem. This is due to the fact that the set $\mathrm{Ad}_K H_d$ of control variables is invariant under conjugation in K so that an optimal trajectory remains optimal after such a conjugation. Furthermore, by general properties of symmetric spaces (as listed above), the set

$$[\mathrm{Ad}_K U_F] = \{[kU_F] \in G/K | k \in K\} \subseteq G/K$$

has nonempty intersection with $[T] \subseteq G/K$, where T is a maximal torus in G. Namely, it holds that

$$[\mathrm{Ad}_K U_F] \cap [T] = [\exp(W_{\mathrm{aff}}X)]$$

for any $X \in \mathfrak{h}$ with $[\exp(X)] \in [\mathrm{Ad}_K U_F]$. Here W_{aff} denotes the so-called affine Weyl group for the pair ($\mathfrak{g}$, $\mathfrak{k}$). It is generated by the reflections of root-hyperplanes in $\mathfrak{h}$ and translations along the inverse roots (i.e., the vectors perpendicular to the root-hyperplanes of fixed length equal to 2) which preserve the subspace $\mathfrak{p} \subseteq \mathfrak{h}$. In the case $G/K = \mathbb{RP}^2$ to be considered here, it turns out that (for $U_F = \mathrm{diag}(e^{i\phi}, e^{-i\phi}) \in T \subseteq G$)

$$[\mathrm{Ad}_K U_F] \cap [T] = \{[U_F], [\bar{U}_F]\}.$$

Hence the set $[T] \subseteq G/K$ falls apart into two fundamental domains under the action of W_{aff}. These are

$$[\Omega] = \{[\mathrm{diag}(e^{i\phi}, e^{-i\phi})] | 0 < \phi < \pi/2\}$$

and

$$[\tilde{\Omega}] = \{[\mathrm{diag}(e^{i\phi}, e^{-i\phi})] | -\pi/2 < \phi < 0\}.$$

It remains to solve the control problem for terminal points $[U_F]$ in $[\Omega]$ (respectively its closure $[\bar{\Omega}]$). The time-optimal torus theorem as formulated below states that one can construct time-optimal trajectories between the points [**1**] and $[U_F]$ from those being completely contained in $[\bar{\Omega}]$. It is therefore not possible to reach $[U_F]$ any faster by leaving $[\bar{\Omega}]$. Now the admissible paths in $[\bar{\Omega}]$ along whose the system can evolve are just concatenations of arcs generated by the elements

$$\mathrm{Ad}_K H_d \cap \mathfrak{h} = \mathbb{O}(H_d)$$

in the Weyl orbit of H_d as introduced above. In our case $\mathbb{O}(H_d) = \{\pm H_d\}$. That is, the Weyl orbit of H_d spans the tangent space of $[T] \subseteq G/K$ at [**1**]. This also holds true for any (generic) $H_d \in [T]$ in the case of a general symmetric space G/K. Thus it becomes evident that any $[U_F] \in [\bar{\Omega}]$ is reachable by a suitable combinations of paths

$$t \mapsto \exp(tY),$$

where $Y \in \mathbb{O}(H_d)$. Since the elements of $\mathbb{O}(H_d) \subseteq h$ commute it is not hard to explicitly determine a time-optimal path joining [**1**] to $[U_F]$. We have thus arrived at the following theorem (which in a different version has first been stated in [8]).

Theorem 3.4. (Time-optimal torus theorem). *We keep the assumptions made throughout this section and Theorem* 3.2. *Denote by $Y_1, \ldots, Y_l$ the elements of the Weyl orbit $\mathbb{O}(H_d)$. Let $\Theta \subseteq \mathfrak{h}$ be a fundamental domain for the action of the affine Weyl group on the Lie algebra $\mathfrak{h}$ (cf.* [3, 6]*), such that $0 \in \bar{\Theta}$. Define $\Omega := \exp(Ad_K\Theta)$ and let $U_F \in \bar{\Omega}$ arbitrary. Then U_F admits the decomposition $U_F = k\exp(Z)k^{-1}$ for some $k \in K$ and a unique $Z \in \bar{\Theta}$. The minimal time $t_{\min}(U_F)$ for steering the adjoint system*

$$\dot{U} = XU, \quad U(0) = \mathbf{1}, \quad X \in \mathrm{Ad}_K H_d \tag{9}$$

to U_F is equal to the smallest non-negative value of α such that one can solve the equation

$$Z = \alpha \sum_{i=1}^{l} \beta_i Y_i \tag{10}$$

with $\beta_i \in \mathbb{R}$ and $\sum_{i=1}^{l} \beta_i = 1$. A trajectory at optimal time $t_{\min}(U_F) = \alpha$ is given by

$$\begin{cases} U(t) = \exp(tkY_jk^{-1}) \prod_{i=1}^{j-1} \exp(\alpha\beta_i kY_ik^{-1}) \\ \alpha \sum_{i=1}^{j-1} \beta_i \le t \le \alpha \sum_{i=1}^{j} \beta_i \\ j = 1, \ldots, l. \end{cases} \tag{11}$$

Proof. See [6].

Corollary 3.5. (Time-optimal control of the reduced system). *Assume the Lie groups G and K to satisfy the prerequisites of Theorem 3.4, let* $\Omega \subseteq G$ *as before and choose* $[U_F] \in G/K$ *arbitrary. Then the set*

$$\mathcal{U}_F := \pi^{-1}([U_F]) \cap \bar{\Omega} \subseteq G \tag{12}$$

is nonempty. Furthermore, the projection under $\pi : G \longrightarrow G/K$ *of any trajectory of type* (11) *with endpoint* $P_F \in \mathcal{U}_F$ *yields a time-optimal trajectory between* $[\mathbf{1}]$ *and* $[U_F]$ *for the reduced system* (4).

Proof. See [3].

We finally describe how the combination of Equivalence Theorem 2.3 with Corollary 3.5 may be used to solve the time-optimal control problem for the unreduced system (2) we were originally interested in. We therefore keep all the assumptions made so far and let $U_F \in G$ be arbitrary. As an easy consequence of Theorem 2.3, it follows that $t_F := t_{\text{inf},1}(U_F)$ equals $t_{\text{inf},3}([U_F])$. Corollary 3.5 can now be used as follows to construct a trajectory $t \mapsto U(t)$ for system (2), which satisfies the time-optimality condition $U(t_F) = U_F$.

(1) Decompose U_F as

$$U_F = k_1 \exp(Z) k_1^{-1} k_2$$

with $k_1, k_2 \in K$ and $Z \in \bar{\Theta}$, where Θ is as defined in Theorem 3.4. By definition of Θ, the term Z in this decomposition is uniquely determined.

(2) Set

$$V_F := k_1 \exp(Z) k_1^{-1} \in \bar{\Omega},$$

where $\Omega \subseteq G$ is as defined in Theorem 3.4. Let $t \mapsto V(t)$, $t \in [0, t_F]$, be a trajectory for system (3) of type (11) such that $V(t_F) = V_F$ holds. By Corollary 3.5, such a trajectory exists and is time-optimal.

(3) By construction, the trajectory $t \mapsto V(t)$ consists of a finite number of arcs of the form

$$t \mapsto k_1 \exp(tY_{j+1}) k_1^{-1} V(t_j),$$
$$t \in [t_j, t_{j+1}],$$

where $k_1 \in K$ is as described in the preceding step, $Y_j \in \mathbb{O}(H_d)$, and $[t_j, t_{j+1}]$ is a subinterval of $[0, t_F]$ as specified in Theorem 3.4. Write Y_j as $k_3 H_d k_3^{-1}$ for some $k_3 \in K$.

(4) Set $\tau_{j+1} := t_{j+1} - t_j$. System (2) can be steered from $V(t_j)$ to

$$V(t_{j+1}) = k_2 \exp(\tau_{j+1} Y_{j+1}) k_2^{-1} V(t_j)$$

within time τ_{j+1} by first producing the element $(k_2k_3)^{-1}V(t_j)$ within zero infimizing time. Evolution under the influence of the drift operator H_d for time τ_{j+1} transfers the system in a second step from $(k_2k_3)^{-1}V(t_j)$ to $\exp(\tau_{j+1}H_d)(k_2k_3)^{-1}V(t_j)$. The point $V(t_{j+1})$ is finally reached from $\exp(\tau_{j+1}H_d)(k_2k_3)^{-1}V(t_j)$ within zero infimizing time.

(5) The iteration of such so-called pulse-drift-pulse sequences as described before transfers the unreduced system (2) within infimizing time t_F from $V(0) = \mathbf{1}$ to V_F. The point $U_F = V_F k_2$ differs from U_F by only an element of K and thus can also be reached within infimizing time t_F.

4. EXAMPLE

We want to illustrate Theorem 3.4 in the model case of the two-particle system with Hamiltonian

$$H(v) = H_d + v_1\sigma_x \otimes I + v_2\sigma_y \otimes I + v_3 I \otimes \sigma_x + v_4 I \otimes \sigma_y.$$

Here I is the 2×2 identity matrix and $\sigma_i \in \mathfrak{su}(2)$, $i \in \{x, y, z\}$ denote the spin matrices with commutator relations $[\sigma_i, \sigma_j] = 2\epsilon_{ijk}\sigma_k$.

The subalgebra $\mathfrak{k} \subseteq \mathfrak{su}(2) \otimes \mathfrak{su}(2)$ spanned by the control Hamiltonians $\sigma_x \otimes I$, $\sigma_y \otimes I$, $I \otimes \sigma_x$, $I \otimes \sigma_y$ is

$$\mathfrak{k} = (I \otimes \mathfrak{su}(2)) \oplus (\mathfrak{su}(2) \otimes I).$$

Its dimension is $\dim \mathfrak{k} = 6$. It is easily checked that the linear span $\mathfrak{p}$ of

$$\sigma_i \otimes \sigma_j, \quad i, j \in \{x, y, z\}$$

together with the subalgebra $\mathfrak{k}$ satisfies the conditions of Definition 3.1. Therefore the pair $(\mathfrak{g}, \mathfrak{k})$ is symmetric.

We may assume that the drift Hamiltonian H_d is contained in the maximal abelian subalgebra $\mathfrak{h} \subseteq \mathfrak{p}$ with basis

$$H_1 = \sigma_x \otimes \sigma_x, \quad H_2 = \sigma_y \otimes \sigma_y, \quad H_3 = \sigma_z \otimes \sigma_z.$$

The convex hull $\mathscr{C}\mathbb{O}(H_d)$ of a typical orbit $\mathbb{O}(H_d)$ is the polytope as illustrated in Fig. 2.

Now let U_F be an arbitrary element chosen from the maximal torus $A := \exp\mathfrak{h} \subseteq G$. To solve the control problem (2) with that U_F as the prescribed terminal state reduces to the problem of finding a point Z_0 in the lattice

$$L := \log(KU_FK) \cap \mathfrak{h} := \{X \in \mathfrak{h} \mid \exp(k_1Xk_2)\} = U_F$$

for some $k_1, k_2 \in K$ which minimizes the function

$$\alpha(Z) := \frac{\|Z\|}{\|\hat{Z}\|}$$

within all $Z \in L$. Here $\hat{Z}$ denotes the unique intersection point of the half-line $\mathbb{R}^+Z$ with the boundary of $\mathscr{C}\mathbb{O}(H_d)$. Thus the problem of finding a time-optimal control is reduced to that of finding a minimal α on the discrete set L. This α then is the minimizing time

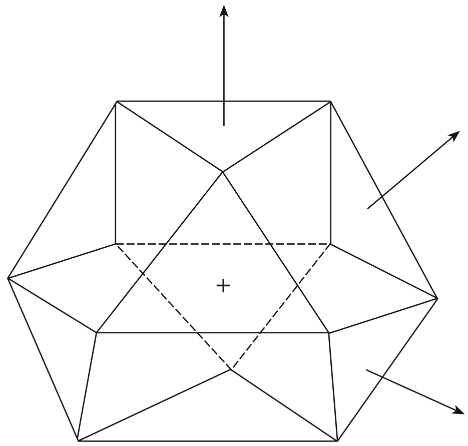

Fig. 2. The convex hull $\mathcal{CO}(H_d)$ of a typical Weyl orbit in the maximal abelian subalgebra $\mathfrak{h}$. The reduced system (4) may evolve at constant speed $\|H_d\|$ in direction of any point in the boundary of the polytope $\mathcal{CO}(H_d)$.

needed for transferring the system from $\mathbf{1} \in G$ to U_F. Writing $\hat{Z}_0$ as

$$\hat{Z}_0 = \sum_{i=1}^{12} \beta_i X_i, \quad X_i \in \mathbb{O}(X_d), \quad \sum_{i=1}^{12} \beta_i = 1,$$

we obtain an explicit description of the corresponding time-optimal trajectory as in (11).

5. CONCLUSIONS

Control systems of type (I), which are the focus of this paper, arise in the field of quantum physics in the context of nuclear magnetic resonance (NMR) and quantum computing. In such situations one is often confronted with the problem of finding optimal control strategies for those systems of coupled spin particles.

We have approached this type of problem from a geometric angle by rephrasing it as a control task on a compact homogeneous space G/K (4). Taking the single particle system as a guiding example, we demonstrated how to explicitly construct time-optimal trajectories between [$\mathbf{1}$] and any given terminal point $[U_F] \in G/K$ under the hypothesis that G/K carries the structure of a Riemannian symmetric space. Evidence was given that optimal trajectories can be chosen to lie entirely within (the projection to G/K of) a maximal torus T of G and are concatenations of arcs with generators in the Weyl orbit $\mathbb{O}(H_d)$ of the fixed drift Hamiltonian H_d. Since these generators are pairwise commuting (in sharp contrast to those of the original problem) the solution can be given by an explicit formula (11).

We also discussed how optimal trajectories for the unreduced system (2) on G can be derived from those of the reduced system (4) on G/K, for any given terminal point $U_F \in G$.

To illustrate our geometric approach to time-optimal control of spin systems, we worked out the particular case of a two-particle system. Although the number of examples where the theory developed so far can be successfully applied is limited through the requirement that G/K be Riemannian symmetric, we nevertheless expect that a geometric approach to similar types of control problems arising in a quantum mechanical context will lead to significant results. Pursuing this line of research further, one might therefore hope to arrive at optimal control strategies in more general settings.

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