# Geometric Control of Quantum Spin Systems

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## 1 Executive Summary

Quantum computers have great theoretical promise in applications of vital interest. However, construction of a useful quantum computer is not yet practical and faces many technical challenges, such as the need to prevent quantum decoherence from corrupting the desired evolution of a quantum spin system.

Khaneja, Brockett and Glaser [5], [6] have described an optimal control strategy for a nuclear magnetic resonance (NMR) quantum spin system with two or three spins. Their methods, however, do not apply directly to systems with more than three spins. We propose to extend their results using differential geometric methods which can be applied to NMR quantum systems with any finite number of spins. The need for control of multi-spin systems is also shared by solid-state methods [1], [9], so this problem has more general application than a particular physical implementation.

## 2 Introduction

The possible uses of quantum computation are of great interest to the United States Army and other branches of government. For example, Shor's factoring algorithm for quantum computers [12] finds the prime factors of a composite number more efficiently than any known algorithm for classical computers. Since the difficulty of factoring large numbers is crucial to the security of many encryption schemes, this is an application of vital interest.

Although the theory of quantum computing algorithms is flourishing (see for example [7], [9]), construction of a useful quantum computer is not yet possible.

One challenge concerns the difficulty of preventing quantum decoherence from corrupting the desired evolution of a system. In the only physically realized scheme to date, nuclear magnetic resonance (NMR), control inputs are mediated by radio-frequency (rf) pulses, and to avoid decoherence it is desirable to make these pulse trains as short and efficient as possible.

Two recent papers by Khaneja, Glaser and Brockett [5], [6] reduce the problem of finding efficient pulse trains for a two-spin or three-spin NMR system to the problem of finding sub-Riemannian geodesics in a quotient space of $SU(4)$. However, the methods they use are not scalable to systems with more than three spins. In this paper we outline a way to extend their results to systems with more than three spins by using geometric methods that were used in the first author's Ph.D. thesis [8] to find sub-Riemannian geodesics of Engel manifolds.

# 3 NMR spin systems and optimal control

## 3.1 NMR systems as control systems

In non-relativistic quantum mechanics the state vector $|\psi(t)>$ of a quantum system at time $t$ is given by

$$|\psi(t)>= U(t)|\psi(0)> \tag{1}$$

where $|\psi(0)>$ is the initial state and the unitary propagator $U(t)$ evolves according to the time-dependent Schrödinger equation

$$\dot{U}(t) = -\frac{\mathrm{i}}{\hbar}H(t)U(t) \tag{2}$$

where $U(0) = I$ (the identity matrix) and $H$ is the Hamiltonian of the system [11].

The Hamiltonian for an NMR system can be decomposed as

$$H = H_d + \sum_{j=1}^{m} u_j H_j \tag{3}$$

where $H_d$ is the *drift* Hamiltonian corresponding to internal couplings, the $u_j$ are *controls*, and the $H_j$ are the *rf* or *control* Hamiltonians which can be externally affected [5]. By (1) and (2) the evolution of a quantum spin system with $n$ spins can be regarded in terms of the action of a one-parameter subgroup $U : \mathbb{R} \to G$ on the space of state vectors $|\psi>$, where $G$ is the unitary matrix group $SU(2^n)$. The problem of finding the most efficient rf pulse train needed to evolve the system to a desired state is therefore equivalent to the problem of finding a time-optimal path from $U(0) = I$ to a desired $U_F$. The control Hamiltonians $H_j$ can be chosen so that the Lie subalgebra generated by $\{\, \mathrm{i}H_j \,\}$ is the Lie algebra of a closed subgroup $K \subset SU(2^n)$.

As explained in [6], the controls $u_j$ can be made so large that the time needed to transition between two elements $U_A$, $U_B$ in the same coset $KU_A = \{\, kU_A :$

$k \in K\}$ is negligible, i.e., so small that the system hardly evolves under the internal Hamiltonian $H_d$ in that time. The problem of finding a time-optimal path between any two elements $U_1, U_2 \in G$ thus reduces to the problem of finding the shortest path from $KU_1$ to $KU_2$ in the coset space $G/K$–an optimal control problem on a homogeneous space.

By equation (3) all admissible motions in $G/K$ are generated by the drift Hamiltonian $H_d$. To choose an initial direction in $G/K$ it suffices to select an appropriate $k \in K$ by means of the controls [6]. In practice, at each point $KU_\alpha \in G/K$, only a proper subspace $D_{KU_\alpha}$ of the directions generated by $H_d$ can be selected by the controls. This constraint might seem to restrict the reachable set of elements of $G/K$, but if the vector fields locally spanning the subspaces $D_{KU_\alpha}$ are *bracket-generating* (see below), a theorem due to Chow [3] guarantees that every point in $G/K$ can be reached from any given starting point by a piecewise smooth path determined by the controls. If an inner product is defined smoothly on the subspaces $D_{KU_\alpha}$, the space $G/K$ is called a *sub-Riemannian manifold*, as defined below. This inner product induces a length functional on the space of admissible paths, and the critical paths of this functional are called *sub-Riemannian geodesics*.

## 3.2 Sub-Riemannian geometry

The notion of a *sub-Riemannian manifold* provides a natural setting for control systems like the one described above.

**Definition 1** *Let $M$ be a smooth manifold and let $D \subset TM$ be a smooth $k$-plane field on $M$, where $k \leq dim\ M$. The* $n$th derived space *of $D$ is defined inductively for $n \geq 0$ by*

$$D^0 = D$$
$$D^n = D^{n-1} + [D^{n-1}, D^{n-1}] \text{ for } n \geq 1$$

*where $[\,,\,]$ denotes the Lie bracket.*

**Definition 2** *A $k$-plane field $D \subset TM$ is* bracket-generating *if, given any point $p \in M$, there is an integer $n \geq 0$ (which may depend on $p$) so that $D_p^n = T_pM$. (This is also known as* Hörmander's condition.*)*

For many problems in control theory, the time derivative of the state vector of a system is constrained to lie in a $k$-plane field $D$ on the *state space* $M$. In the NMR quantum control problem considered here, the state space is $M = G/K$ and $D$ is the collection of subspaces $\{D_{KU_\alpha} | KU_\alpha \in G/K\}$. When $D$ is bracket-generating, as it is here, the following theorem of Chow implies that the controls allow the system to reach any desired endstate from any initial state. First, another definition is needed.

**Definition 3** *Let $M$ be a smooth manifold with a smooth $k$-plane field $D \subset TM$. A curve $\gamma : [a, b] \to M$ is called* admissible *if, whenever $\dot{\gamma}(t)$ exists, $\dot{\gamma}(t) \in D_{\gamma(t)}$.*

**Theorem 1** (Chow, 1935) *Let $D \subset TM$ be a smooth $k$-plane field on a connected manifold $M$. If $D$ is bracket-generating, then given any two points $p, q \in M$, there is a piecewise-smooth admissible curve $\gamma : [a, b] \to M$ with $\gamma(a) = p$, $\gamma(b) = q$.*

PROOF. See [3] for a proof. □

Given a connected manifold $M$ with a bracket-generating $k$-plane field $D \subset TM$, by Chow's theorem any two points of $M$ are connected by at least one admissible curve, so it is of interest to define the length of such a curve. Of special interest is the case where the length of a vector in $D$ is defined by an inner product called a *sub-Riemannian metric*.

**Definition 4** *Let $D \subset TM$ be a $k$-plane field. A* sub-Riemannian metric *on $D$ is an inner product $\langle\, , \rangle$ defined smoothly on the fibers of $D$.*

**Definition 5** *Let $M$ be a connected manifold with a bracket-generating $k$-plane field $D \subset TM$ equipped with a sub-Riemannian metric $\langle\, , \rangle$.*

1. *The* sub-Riemannian length *of a smooth admissible curve $\gamma : [a, b] \to M$ is*
$$\mathcal{L}(\gamma) = \int_a^b \langle \dot{\gamma}(t), \dot{\gamma}(t) \rangle^{1/2}\, dt \tag{4}$$
*If $\gamma$ is piecewise-smooth, the length of $\gamma$ is the sum of the lengths of its smooth segments.*

2. *Let $p, q \in M$ be any two points in $M$. The* sub-Riemannian distance *between $p$ and $q$ is*
$$d(p, q) = \inf\{\mathcal{L}(\gamma) | \gamma : [a, b] \to M \text{ admissible with } \gamma(a) = p, \gamma(b) = q\} \tag{5}$$

3. *The triple $(M, D, \langle\, , \rangle)$ is called a* sub-Riemannian manifold.

If an admissible path $\gamma$ connecting $p$ and $q$ with $\mathcal{L}(\gamma) = d(p, q)$ exists, $\gamma$ is called a *sub-Riemannian minimizer*. Critical points of (4) are called *sub-Riemannian geodesics*. Every sub-Riemannian minimizer is a geodesic, but the converse is not true; however, every sub-Riemannian geodesic is a *local* minimizer. Thus searches for minimizers often begin by computing geodesics.

## 3.3 Optimal control of NMR spin systems

Returning to the quantum control problem above, finding an optimal path between two elements of the coset space $G/K$ amounts to finding a sub-Riemannian minimizer. In [5] the authors find sub-Riemannian geodesics of $\frac{SU(4)}{SU(2) \otimes SU(2)}$, corresponding to the two-spin case (and extended to the three-spin case in [6]). Their computations take advantage of the fact that $\frac{SU(4)}{SU(2) \otimes SU(2)}$ is a Riemannian symmetric space. However, for systems with a higher number of spins $G/K$ is

no longer a Riemannian symmetric space [5]. The problem of finding explicit solutions for time-optimal paths in higher spin systems is still open, and would benefit from a method that is more generally applicable.

Such a method already exists: the *Griffiths formalism*, named for the author of [4]. In [8] the first author employed the Griffiths formalism to find the equations of sub-Riemannian geodesics on Engel four-manifolds, and found explicit solutions for sub-Riemannian geodesics on the Lie groups $SO(3) \times S^1$, $SEuc(2) \times S^1$, and $SO(2,1) \times S^1$. Roughly speaking, in the Griffiths formalism one finds critical points of constrained variational problems on a manifold $M$ by lifting the geodesic equations to a covering space defined by the linear constraints. The constrained variational problem on $M$ is thus lifted to an unconstrained problem on this covering space and solutions project down to solutions of the original problem on $M$. The method does not depend on any special properties of $M$, such as whether $M$ is a symmetric space.

We propose to find time-optimal paths for at least one system of more than three spins, using the Griffiths formalism and other methods from the theory of exterior differential systems. The symmetries of the homogeneous spaces $G/K$ may make it possible, as with the Lie groups investigated in [8], to find these solutions by quadrature, using a generalized form of Noether's theorem (see also [2]).

The need for multi-spin control is not confined to NMR quantum computers, but is shared by a number of solid-state approaches to quantum computer implementation (such as quantum dots) [1],[9]. Thus this problem is not limited to just one means of physical implementation.

The dimension of $G/K$ increases rapidly with the number of spins, so this problem will entail a good deal of computation. The task should be lightened by a computer algebra system such as *Maple 7* but will still be intensive. However, the goal is worthwhile: we need to find ways to control larger numbers of spins and solutions to the time-optimal path problem should be of value in this endeavor.

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