Geometric Control of Quantum Systems–Progress Report

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1 Executive Summary

Quantum computation is a very active area of research with potential 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. Our methods are also applicable to other constrained quantum spin systems.

2 Introduction

Research in the field of quantum computation is extremely active, motivated by the theoretical possibility of constructing quantum machines with unusual capabilities. For example, Shor's factoring algorithm [11] demonstrates that a quantum computer could find 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 the process of decoherence, caused by coupling of the quantum system to the environment, from corrupting the desired evolution of a system. For example, in nuclear magnetic resonance (NMR) experiments, control inputs are mediated by radio-frequency (rf) pulses, and to minimize 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 different method that is, in principle, applicable to a system with any number of spins, and comment on some of the practical difficulties in calculating the desired sub-Riemannian geodesics with this method.

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 [10].

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 the closed subgroup As before, $K = SU(2) \otimes \cdots \otimes SU(2)$ (n factors).

The set of possible velocity vectors (*accessible directions*) in $SU(2^n)$ is

$$Ad_K\,(iH_d) = \{\, k(iH_d)\,k^{-1} \mid k \in K \,\}.$$

This is a proper subspace of the entire tangent space at any point. (The velocity vectors are subject to a non-holonomic constraint.) However, this subspace is *bracket-generating*: that is, at any point $p \in SU(2^n)$ the tangent space is spanned by the iterated Lie brackets of vector fields in $Ad_K\,(iH_d)$. The following theorem shows why this is sufficient for our purposes: any two points in the state space are connected by at least one *admissible* curve γ, that is, a curve whose velocity vectors lie in $Ad_K\,(iH_d)$.

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. □

In the language of control theory, the fact that $D = Ad_K\,(iH_d)$ is bracket-generating implies that the entire state space $SU(2^n)$ is controllable. Moreover, there is a natural generalization of Riemannian geometry that allows us to measure the length of any admissible curve γ.

Definition 1 *A* sub-Riemannian metric *on D is an inner product $\langle\, ,\, \rangle$ defined smoothly on the subspaces lying in D.*

Definition 2 1. *The* sub-Riemannian length *of a smooth admissible curve $\gamma : [a, b] \to SU(2^n)$ is*

$$\mathcal{L}(\gamma) = \int_a^b \langle \dot{\gamma}(t), \dot{\gamma}(t) \rangle^{1/2}\, dt \tag{4}$$

If γ is piecewise-smooth, the length of γ is the sum of the lengths of its smooth segments.

2. *Let $p, q \in SU(2^n)$ be any two points in $SU(2^n)$. The* sub-Riemannian distance *between p and q is*

$$d(p, q) = \inf\{\mathcal{L}(\gamma) | \gamma : [a, b] \to M \text{ admissible with } \gamma(a) = p, \gamma(b) = q\} \tag{5}$$

If an admissible path γ connecting p and q with $\mathcal{L}(\gamma) = d(p, q)$ exists, γ 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.

3.2 A brief description of the Griffiths formalism

The *Griffiths formalism*, named for the author of [4], provides a coordinate-independent method for computing sub-Riemannian geodesics (and other constrained variational problems). Briefly, the Griffiths formalism starts by writing the linear velocity constraints in the tangent bundle as a system of differential 1-forms $\theta^1, \ldots, \theta^m$. These 1-forms define a subbundle of the cotangent bundle over $X = D \times \mathbb{R}$ and we can lift the constrained variational problem on the state space to this higher-dimensional space where it corresponds to an unconstrained variational problem. Solutions to the unconstrained variational problem "upstairs" project onto solutions of the constrained variational problem on state space.

More precisely, let $X = D \times \mathbb{R}$ where $D \subset TM$ is the k-plane field in question. On X we lift the sub-Riemannian energy functional to a 1-form $\phi = 1/2((p^1)^2 + \cdots + (p^k)^2)dt$ and define a submanifold Z of T^*X by

$$Z = \bigcup_{x \in X} \{Z_x\}$$

where for each $x \in X$,

$$Z_x = \{\phi(x) + I_x \subset T_x^* X\}.$$

where I is the module spanned by the 1-forms θ^i, namely

$$I = \{\lambda_1 \theta^1 + \cdots + \lambda_m \theta^m | \lambda_1, \ldots, \lambda_m \in \mathbb{R}\}.$$

After some more calculations (omitted for brevity) one obtains a system of ordinary differential equations in the variables λ_i. Solutions to this system are curves in the cotangent space at the identity of $SU(2^n)$; they must be lifted to the entire Lie group in order to find sub-Riemannian geodesics on the group.

One practical difficulty with this method is that the number of differential equations to be solved increases exponentially with the number of spins in the quantum system. The table below illustrates this.

n	unitary group	number of structure eqns
1	$SU(2)$	3
2	$SU(4)$	15
3	$SU(8)$	63
4	$SU(16)$	255
5	$SU(32)$	1023

3.3 Current work in progress

Due to the large number of variables and equations involved, we have started with the case $n = 2$ as a test case and also for comparison with the calculations in [5] and [6]. Even in this case there is still work to be done; in particular,

lifting the solutions in cotangent space to the full state space involves some ingenuity.

As we become more familiar with the symmetries involved in this problem, quicker solution methods may become apparent. However, at present there are many man-hours involved in simply determining the geodesic equations.

4 Conclusion

The need for multi-spin control through constrained control mechanisms is not confined to NMR quantum computers, but is shared by other quantum control problems. Thus this problem is not limited to just one means of physical implementation.

The problem we are currently investigating entails a good deal of computation. The task should be lightened by software such as *Maple 7* and *Matlab* but will still be labor-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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