Geometric Control of Quantum Spin Systems: The Three-Spin Chain Problem and Beyond

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1 Executive Summary

In 1997 Peter Shor showed that a quantum computer would be able to factor numbers exponentially faster than a classical computer [15]. Since the difficulty of factoring large numbers is crucial to several widely used encryption schemes, quantum computation is of great interest to the United States Army and other government agencies. However, although some experiments have succeeded in implementing quantum computation for special problems with a small number of quantum bits ("qubits"), it is not yet known whether quantum computers can be built on a more practical scale. In particular, interaction of a quantum system with its environment can corrupt the desired evolution of the system– a phenomenon known as "decoherence." Minimizing decoherence is therefore crucial in the design of any quantum computational system.

One method of minimizing decoherence is to perform quantum operations in a time-optimal manner. Khaneja, Brockett and Glaser [8], [9] have designed and implemented time-optimal controls for a nuclear magnetic resonance (NMR) quantum spin system with two qubits. Time-optimal control for the general case of three or more qubits is still an unsolved problem.

This paper reports a partial solution to a time-optimal quantum control problem for an NMR three-spin chain system, progress towards a complete solution, and also progress in solving the general NMR time-optimal control problem for three and four spins.

2 Time Optimal Control of NMR spin systems

2.1 NMR systems as control systems

In non-relativistic quantum mechanics the evolution of the wave function $|\psi(t)>$ of an n-qubit quantum system at time t is given by

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

where $|\psi(0)>\in \mathbb{C}^{2^n}$ is the initial wave function and the unitary operator $U(t) \in SU(2^n)$ 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 $H(t)$ is the Hamiltonian of the system at time t [14].

In controlled quantum systems the Hamiltonian H is a function of control inputs u_j as well as time. However, since the control inputs themselves can be regarded as functions of time, the time-optimal control problem can be written as a time-dependent problem. The quantum optimal control problem is to generate a desired unitary operator U_F in the least possible time. By (1) and (2), the problem of finding a time-optimal path from $U(0) = I$ to U_F amounts to finding time-varying controls $u_j(t)$ so that the resulting path $U(t)$ defined by (2) is as short as possible, in a sense that will be defined in what follows.

Although the general state space for an n-qubit quantum control problem is the Lie group $SU(2^n)$, the state space can often be reduced to a quotient of this group. Such is the case with the first problem below.

2.2 Problem 1: Optimal Control of a Three-Spin Chain

A three-spin chain is a system of three nuclear spins situated at roughly equal intervals along a straight line. The complete state space for this system is $SU(8)$, but the optimal control problem can be reduced to finding a time-optimal path in $SO(4)$. The equation of the control system in this reduced state space is

$$\begin{aligned} \dot{\gamma}(t) &= (u_1(t)X_1 + u_2(t)X_2 + u_3(t)X_3)\gamma(t) \\ \gamma(0) &= I \end{aligned} \tag{3}$$

where $\gamma(t) \in SO(4)$ for each t, $u_1(t), u_2(t), u_3(t)$ are the controls and

$$X_1 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, X_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

$$X_3 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

are linearly independent elements of the Lie algebra $so(4)$.

The following interpretation of equation (3) is useful. Let $\gamma : [a, b] \to SO(4)$ be a piecewise smooth solution curve of (3) generated by some choice of control functions u_j. Then equation (3) states that if the velocity vector $\dot{\gamma}(t_0)$ exists, it must lie in a certain three-dimensional vector space based at $\gamma(t_0)$, namely

$$\dot{\gamma}(t_0) \in \text{ span } \{X_1\gamma(t_0), X_2\gamma(t_0), X_3\gamma(t_0)\}.$$

2.2.1 Controllability

Let D be the 3-plane field (or *distribution*) on $SO(4)$ defined at each point $\gamma \in SO(4)$ by

$$D_\gamma = \text{ span } \{X_1\gamma, X_2\gamma, X_3\gamma\}; \tag{4}$$

that is, $D \subset TSO(4)$ is the 3-plane field consisting of right translations of span $\{X_1, X_2, X_3\}$. Then the above interpretation of (3) can be summarized by stating that every smooth solution curve of (3) is tangent to D. This 3-plane field has the following property.

Definition 1 *Let D be a k-plane field on a smooth manifold M with dimension $m \geq k$. D is called* bracket-generating *if at each point $p \in M$, iterated Lie brackets of the vector fields locally spanning D in a neighborhood of p span the tangent space T_pM.*

It is easy to check that D is a bracket-generating 3-plane field. By a theorem due to Chow, this has a useful consequence for the control system defined by (3). To explain this, we need another definition.

Definition 2 *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 [4] for a proof. □

Since the state space in question, $SO(4)$, is a connected manifold, it follows that the any desired final state $\gamma_F \in SO(4)$ can be reached from the identity I by a piecewise control curve $\gamma : [a, b] \to SO(4)$ whose smooth components are tangent to D, that is, a curve that obeys the equation (3). In the language of control theory, the system is *controllable*: that is, any desired final state can be reached from the initial state using the controls u_j.

2.2.2 Time-Optimal Controls for the Three-Spin Chain

The time-optimal control problem is to find an admissible curve $\gamma : [a, b] \to SO(4)$ that locally minimizes a quadratic length functional, called a *sub-Riemannian metric*, defined on admissible curves as follows.

Definition 3 *Let M be a smooth manifold equipped with a bracket-generating k-plane field D.*

1) *A smooth inner product $\langle\, , \rangle$ on the fibers of $D \subset TM$ is called a* sub-Riemannian metric.

2) *The* sub-Riemannian length *of a smooth admissible curve $\gamma : [a, b] \to M$ is*

$$\mathcal{L}(\gamma) = \int_a^b \sqrt{\langle\, \dot{\gamma}(t), \dot{\gamma}(t)\, \rangle}\, dt. \tag{5}$$

(If γ is piecewise-smooth, extend this definition in the obvious manner.)

3) *The* sub-Riemannian distance *between two points p and q in an Engel manifold is*

$$\mathcal{D}(p, q) = \inf\{\mathcal{L}(\gamma) : \gamma \textit{ is a admissible curve connecting } p \textit{ and } q\,\}$$

The problem of finding time-optimal controls for the system (3) is equivalent to the problem of finding sub-Riemannian geodesics for the length functional (6) where D is the 3-plane field defined above in (4). In local coordinates this functional has the form

$$\mathcal{L}(\gamma) = \int_a^b \sqrt{p_1^2 + p_2^2 + p_3^2}\, dt, \tag{6}$$

where p_i is the component of $\dot{\gamma}(t)$ in the X_i direction, for $i = 1, 2, 3$.

The admissible curves γ of the system (3) are subject to the linear velocity constraints encoded by the 3-plane field D, so it is *a priori* possible that some admissible curves do not admit any nontrivial C^1 variations (see [3] for the conditions under which this occurs). In such a case the admissible curve is called *rigid* and the usual methods of finding geodesics through variational vector fields cannot be used. However, when a sub-Riemannian geodesic is *regular* (that is, not rigid) a method for solving constrained variational problems called the *Griffiths formalism* may be used. The interested reader may refer to [6] for a description of this method; the papers [2] and [5] contain specific uses of the griffiths formalism.

In this paper the details of the Griffiths formalism calculation for the three-spin chain problem are omitted for the sake of brevity. However, the result of

the calculation is that the *Euler system* of the regular geodesics is

$$\begin{aligned}
\dot{\lambda_1} &= \lambda_2\lambda_4, \\
\dot{\lambda_2} &= \lambda_3\lambda_6 - \lambda_1\lambda_4, \\
\dot{\lambda_3} &= -\lambda_2\lambda_6, \\
\dot{\lambda_4} &= \lambda_3\lambda_5, \\
\dot{\lambda_5} &= -\lambda_3\lambda_4 + \lambda_1\lambda_6, \\
\dot{\lambda_6} &= -\lambda_1\lambda_5. \qquad (7)
\end{aligned}$$

By inspection, the following are conserved quantities of the system (7):

$$\lambda_1^2 + \lambda_2^2 + \lambda_3^2 = C_1, \qquad (8)$$

$$\lambda_4^2 + \lambda_5^2 + \lambda_6^2 = C_2, \qquad (9)$$

$$\lambda_1\lambda_3 - \lambda_4\lambda_6 + \lambda_2\lambda_5 = C_3, \qquad (10)$$

where C_1, C_2 and C_3 are constants. By the general theory elaborated in [2], solution curves of the Euler system (7) lie on coadjoint orbits in the cotangent space $so(4)^*$. The conservation laws (8), (9) and (10) bring the problem down to a 3-dimensional submanifold of $so(4)^*$.

The system (7) is amenable to numerical solution (for example, the standard Runge-Kutta 4th-order algorithm in *Maple V* is stable on (7)), and solutions to (7) may be lifted to the Lie group $SO(4)$ via a generalization of Noether's theorem [2]. In that sense the problem of finding optimal controls has been solved.

However, these solutions are not convenient for use by experimenters. The best possible solution would be a closed-form solution for $\lambda_1, \ldots, \lambda_6$, depending on boundary conditions. The current strategy is to exploit the canonical symplectic form on the coadjoint orbits and also on $so(4)^*$ to obtain additional conservation laws; work continues on this problem and results will be announced in the spring of 2006.

2.3 Time-optimal control of more general NMR spin systems

The general time-optimal control problem for an n-qubit NMR system is to find optimal solution curves for equation (2)

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

where $U(t)$ takes values in the state space $SU(2^n)$. The general Hamiltonian for an NMR system can be written as

$$H(t) = H_d + \sum_{j=1}^{m} u_j(t)H_j \qquad (11)$$

where H_d is the *drift* Hamiltonian corresponding to internal couplings, the $u_j(t)$ are time-varying *controls*, and the H_j are the *rf* or *control* Hamiltonians which can be externally affected [8]. Since the state space $SU(2^n)$ is a compact Lie group, the system is controllable if the iterated Lie brackets of $\{H_d, H_1, \ldots, H_m\}$ generate the Lie algebra $su(2^n)$ [7]. Note carefully, however, that since the drift term is uncontrolled, the solution curves of (2) are tangent to a field of *affine* planes, not a distribution.

The presence of the nonzero drift term therefore means that the time-optimal geometry is not, in general, sub-Riemannian. The two-qubit case is a special exception. In [8] Khaneja, Brockett and Glaser showed that for a two-qubit NMR system, the state space can be reduced to $\frac{SU(4)}{SU(2)\otimes SU(2)}$. This reduced space is a Riemannian symmetric space, and their analysis exploited this fact to find optimal solutions using the methods of sub-Riemannian geometry.

For higher numbers of qubits the coset space is not a symmetric space. In principle, the Pontryagin Maximum Principle [13] can be applied to these problems. For the general four-qubit problem, the complete state space $SU(16)$ has dimension $2^{16} - 1 = 255$, so *a priori* this is a computationally intensive task. For this problem the following general plan will be followed:

- examine ways in which the state space may be reduced, perhaps to the coset space
$$S = \frac{SU(16)}{\bigotimes_1^4 SU(2)};$$
- apply the Pontryagin Maximum Principle and methods from exterior differential systems to find optimal paths;
- find numerical solutions;
- search for closed-form solutions for path planning (more difficult).

A full report on this problem will also be issued in the spring of 2006.

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