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

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Geometric Quantum Control

- Quantum control is
  - a new and growing field of research;
  - necessary if we are to build **quantum computers**.
- *Geometric* quantum control is
  - an application of "pure" mathematics to quantum control problems;
  - the natural setting for *optimal* control of quantum spin systems.
- This presentation reports a partial solution to one quantum optimal control problem, progress towards a complete solution, and a strategy for solving more general quantum control problems.

Why are quantum computation and information worth the effort?

- P. Shor (1994) found a quantum algorithm for factoring integers that is exponentially faster than any known classical algorithm.
- Factoring large integers is crucial to decrypting modern codes such as RSA.
- Quantum information channels can be constructed so that any eavesdropping is always detected.

Examples of quantum computation / information research

- Dr. Howard Brandt, ARL Adelphi: quantum optics and quantum communications
- Dr. Herschel Rabitz's group at Princeton: quantum optics, multi-level encoding of qubits
- Dr. David Cory's group at MIT: nuclear magnetic resonance (NMR) control, quantum error correction
- Dr. Isaac Chuang's group at the MIT Media Lab: NMR quantum computing (implemented Shor's algorithm)
- Dr. Navin Khaneja at Harvard: time-optimal NMR quantum control

A brief overview of quantum computers

- smallest unit of data is the *qubit*
- qubits can be physically encoded as quantum states; for example, spin states.

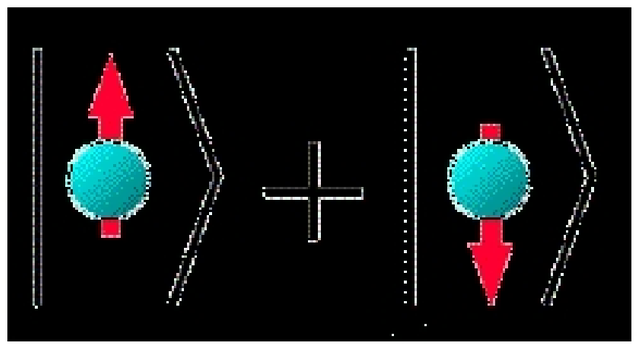

Figure 1: Spin up and spin down states

A brief overview of quantum computers, continued

The *wave vector* $|\psi>$ for a 1-qubit quantum system is a linear combination (or *superposition*) of the basic "up" and "down" vectors $|0>$ and $|1>$:

$$|\psi> = \alpha|0> + \beta|1> \text{ where}$$

$$|0> = \begin{bmatrix} 1 \\ 0 \end{bmatrix},$$

$$|1> = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

By the general theory of quantum mechanics, α and β are complex numbers so that $\sqrt{|\alpha|^2 + |\beta|^2} = 1$.

A brief overview of quantum computers, continued

- Classical computers perform calculations via Boolean operators such as AND, OR and NOT gates acting on bits with values 0 and 1.
- Quantum computers perform calculations via *unitary* operators acting on qubits with values $\alpha|0> + \beta|1>$.
- Example: the X gate

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$X(\alpha|0> + \beta|1>) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix}.$$

A brief overview of quantum computers, continued

Another example–the Hadamard gate: $H = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.

$$H(\alpha|0> + \beta|1>) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \frac{\alpha+\beta}{\sqrt{2}} \\ \frac{\alpha-\beta}{\sqrt{2}} \end{bmatrix}$$

$$= \alpha \frac{|0> + |1>}{\sqrt{2}} + \beta \frac{|0> - |1>}{\sqrt{2}}$$

A brief overview of quantum computers, continued

The X gate, Hadamard gate, and other quantum 1-qubit gates are *unitary* operators.

- U is a unitary operator if it leaves the amplitude $\sqrt{|\alpha|^2 + |\beta|^2}$ of a 1-qubit wave function unchanged: this preserves the information encoded in the qubit.
- Equivalently, U is unitary if $U^*U = I$ (the identity matrix).
- The group of unitary operators on 1-qubit wave functions with determinant 1 is $SU(2)$.
- The group of unitary operators on n-qubit systems is $SU(2^n)$.

Decoherence

An ideal quantum computer would perform only unitary operations on n-qubit wave functions until the result of a calculation is needed.

However, quantum systems inevitably interact with their environment, and this interaction can corrupt the desired evolution of the n-qubit wave function–a phenomenon called *decoherence* (or, sometimes, *quantum noise*).

Successful implementation of a quantum computer will require ways to minimize decoherence or mitigate its effects on the encoded data.

Minimizing decoherence

- One method for minimizing decoherence: perform the desired unitary operations as quickly as possible within physical limits.
- This requires *time-optimal control* of the quantum system.
- This presentation will focus on two time-optimal control problems for NMR quantum systems.

The general n-qubit optimal control problem

Let $|\psi(t)>\in \mathbb{C}^{2^n}$ be the wave vector at time t for an n-qubit quantum system. The wave vector evolves according to the equation

$$|\psi(t)>= U(t)|\psi(0)>$$

where $|\psi(0)>$ is the initial wave function and the unitary operator $U(t) \in SU(2^n)$ evolves according to the time-dependent Schrödinger equation

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

where $U(0) = I$ (the identity matrix) and $H(t)$ is the Hamiltonian of the system at time t.

The general n-qubit optimal control problem, continued

$$\begin{aligned} \dot{U}(t) &= -\frac{\mathrm{i}}{\hbar} H(t) U(t) \\ U(0) &= I \end{aligned} \tag{1}$$

Solution curves $U : [a, b] \to SU(2^n)$ of (1) are paths in the *state space* $SU(2^n)$.

- In controlled quantum systems, the Hamiltonian H is a function of both time t and controls u_j.
- Time-optimal control: choose controls $u_j(t)$ so that the resulting curve $U : [a, b] \to SU(2^n)$ reaches the desired unitary operator U_F in minimum time.
- For many problems it is possible to use a *reduced* state space (e.g. a quotient of $SU(2^n)$).

Problem 1: Optimal Control of the Three-Spin Chain

- Three qubits: three nuclear spins in a one-dimensional array.
- Quantum control system:

$$[\dot{\gamma}_{ij}(t)] = \begin{bmatrix} 0 & u_1(t) & 0 & 0 \\ -u_1(t) & 0 & u_2(t) & 0 \\ 0 & -u_2(t) & 0 & u_3(t) \\ 0 & 0 & -u_3(t) & 0 \end{bmatrix} [\gamma_{ij}(t)] \qquad (2)$$

  where the matrices $[\gamma_{ij}(t)]$ are elements of the reduced state space $SO(4)$, and u_1, u_2 and u_3 are the controls.
- Goal: time-optimal controls $u_1(t), u_2(t), u_3(t)$.

The Three-Spin Chain, continued

Equation (2) can be rewritten as

$$\dot{\gamma}(t) = (u_1 X_1 + u_2 X_2 + u_3 X_3)\gamma(t), \tag{3}$$

where

$$X_1 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, X_2 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, X_3 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix}$$

By a theorem due to Chow (1939), any desired final state $\gamma_F \in SO(4)$ can be reached by a solution curve of (3) starting from the identity.

Time-optimal controls for the three-spin chain

We wish to find solution curves $\gamma : [a, b] \to SO(4)$ with $\gamma(0) = I$ that minimize the energy functional

$$\Phi(\gamma) = \frac{1}{2} \int_a^b u_1^2 + u_2^2 + u_3^2 \, dt \tag{4}$$

Since the solution curves of (3) are tangent to the three-plane field D on $SO(4)$ spanned by right-translations of $\{X_1, X_2, X_3\}$, the computations must use some form of constrained minimization technique. For this calculation the *Griffiths formalism* was used.

Time-optimal controls for the three-spin chain, continued

Result 1: the optimal controls are determined by the following system of nonlinear ODEs in Lagrange multipliers $\lambda_1, \ldots, \lambda_6$, called the *Euler system*:

$$\dot{\lambda_1} = \lambda_2\lambda_4, \quad \dot{\lambda_2} = \lambda_3\lambda_6 - \lambda_1\lambda_4, \quad \dot{\lambda_3} = -\lambda_2\lambda_6,$$
$$\dot{\lambda_4} = \lambda_3\lambda_5, \quad \dot{\lambda_5} = -\lambda_3\lambda_4 + \lambda_1\lambda_6, \quad \dot{\lambda_6} = -\lambda_1\lambda_5.$$

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By inspection this system has three quadratic conservation laws:

$$\lambda_1^2 + \lambda_2^2 + \lambda_3^2 = C_1,$$
$$\lambda_4^2 + \lambda_5^2 + \lambda_6^2 = C_2,$$
$$\lambda_1\lambda_3 - \lambda_4\lambda_6 + \lambda_2\lambda_5 = C_3.$$

Time-optimal controls for the three-spin chain, continued

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The time-optimal solutions are given by $u_1 = \lambda_1, u_2 = \lambda_2, u_3 = \lambda_3$.

Time-optimal controls for the three-spin chain: next steps

- The result just presented allows complete numerical solutions for time-optimal control of the three-spin chain.
- However, experimenters in NMR control want something more: *closed-form* expressions for the controls.
- The three conserved quantities listed above allow the problem to be reduced to finding solutions on a three-manifold. There are geometric reasons to think there should be more conserved quantities, arising from the symmetry of the reduced state space $SO(4)$.
- If closed-form solutions can be found, it would be a breakthrough. Work on this continues.

Problem 2: Optimal Control of More General NMR Quantum Systems

Recall that the control system of a general n-qubit quantum system is given by the Schrödinger equation

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

where the Hamiltonian $H(t)$ is controlled.

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The controlled Hamiltonian for an n-qubit NMR quantum system is

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

where H_d is the *drift* component corresponding to internal couplings, the $u_j(t)$ are time-varying *controls*, and the H_j are the *rf* or *control* components.

Problem 2: Optimal Control of More General NMR Quantum Systems

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

The system is controllable if iterated Lie brackets of $\{H_d, H_1, \ldots, H_m\}$ generate the Lie algebra $su(2^n)$.

The presence of the drift term H_d means that the optimal control problem requires a somewhat different approach, involving Pontryagin's Maximum Principle.

Problem 2: Optimal Control of More General NMR Quantum Systems

- Khaneja, Brockett and Glaser (2001): optimal controls for general 2-qubit NMR systems
- Solution involved using the Pontryagin Maximum Principle on the reduced state space $\dfrac{SU(4)}{SU(2) \otimes SU(2)}$.
- Solutions for $n \geq 3$ qubits still not known
- Progress on $n = 4$ may benefit from recent results in geometric control theory, but work is still in first stages

Summary

- We now can use numerical methods for optimal control of the three-spin chain quantum system (result 1)
- Work continues on finding closed-form solutions to this problem
- Exploration of the 4-qubit case is just beginning
- General methods applicable to other quantum systems, not just NMR control

The goal: to allow more sophisticated experiments in quantum control that will ultimately lead to construction of a practical quantum computer.