

WORKSHOP ON QUANTUM CONTROL THEORY AND ITS APPLICATIONS

Final Report

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Richard Murray Hideo Mabuchi

Control and Dynamical Systems
California Institute of Technology
Pasadena, CA 91125

Abstract

This grant supported a workshop, held at Caltech in August 2004, that brought together experts in quantum mechanics, control theory, and dynamical systems for an exchange of ideas on the analysis, control, and design of quantum systems. One of the major goals of the workshop was to establish substantive technical interactions between physicists working on quantum 'applications' and control and dynamical systems researchers who have insights and tools but lack a concrete sense of what problems are of primary interest. The workshop highlighted anticipated applications of quantum control in quantum information science, control of molecular reactions, and design of electronic and photonic nanostructures. The workshop results are available on the web and documented in a paper that has been submitted to the International Journal of Robust and Nonlinear Control.

A copy of the report generated based on the discussions in the workshop is attached.

Attendees: Claudio Altafini, Axel Andre, Mike Armen, David Awschalom, Jim Beck, Viacheslav Belavkin, Anthony Bloch, Luc bouten, Roger Brockett, Yanbei Chen, doug Cochran, Michel Devoret, andrew Doherty, Milos Drezgic, Fariba Fahroo, JM Geremia, Avishek Ghosh, Steven Girvin, Steffen Glaser, Symeon Grivopoulos, Madalin Guta, Salman Habib, John Hauser, Sharon Heise, Asa Hopkins, Matthew James, Poul Jessen, Andrew Johnson, Raisa Karasik, Navin Khaneja, Robert Kosut, PS Krishnaprasad, Ben Lev, Jr-Shin Li, Daniel Lidar, Hans Maassen, Hideo Mabuchi, Nergis Mavalvala, Gerard Milburn, Tony Miller, Richard Murray, Brent Pryor, Herschel Rabitz, Keith Schwab, Andrew Silberfarb, Jon Sjogren, Jen Sokol, John Stockton, T-J Tarn, Francesco Ticozzi, Ulrike Troppmann, Ramon van Handel, Howard Wiseman, Naoki Yamamoto, Masahiro Yanagisawa, Haidong Yuan, Jun Zhang.

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Agenda

Talks were presented in the Lees-Kubota lecture hall at Caltech in Pasadena, California.

The first two days focused on developing an overview of the field, from theoretical perspectives to experimental challenges and opportunities. During the third and fourth days the emphasis turned to detailed modeling and mathematical methods.

Saturday 21 August

8:00–8:30am	Breakfast and registration
8:30–8:45	Welcoming remarks
8:45–9:30	Navin Khaneja
	<u>Optimal control in magnetic resonance</u>
9:30–10:15	Hideo Mabuchi
	<u>Real-time quantum feedback control of atomic spin-squeezing</u>

10:15–10:30 Coffee break

10:30–11:15	Steffen Glaser
	<u>Exploring the physical limits of quantum evolution in NMR</u>
11:15–12:00pm	Nergis Mavalvala
	<u>Quantum noise in gravitational-wave detectors</u>

12:00–1:30 Lunch

1:30–2:15	Michel Devoret
	<u>Amplifying quantum signals with the bifurcation of a Josephson Junction</u>
2:15–3:00	Steve Girvin
	<u>Quantum optics with electrical circuits: Strong Coupling Cavity QED</u>

3:00–3:30 Break

3:30–4:15	Tzyh-Jong Tarn
	<i>Control and observation of quantum mechanical systems: systems theoretical approach</i>
4:15–5:00	Roger Brockett
	<u><i>Optimal inputs for NMR system identification</i></u>

5:00–5:30 Break

5:30–6:15	Herschel Rabitz
	<u><i>Control of quantum dynamics phenomena: How do the experiments work, Why do they work, and What may lie ahead?</i></u>

6:30–8:30 Opening banquet

Sunday 22 August

8:30–8:45	Aims of the workshop
8:45–9:30	Salman Habib
	<u><i>Quantum feedback control in nanomechanics</i></u>
9:30–10:15	Keith Schwab
	<i>Progress to feedback-cool a nano-mechanical resonator under continuous, near-quantum-limited position measurement</i>

10:15–10:30 Coffee break

10:30–11:15	Ulrike Troppmann
	<u><i>Molecular quantum computing: an optimal control approach</i></u>
11:15–12:00pm	David Awschalom

	<i>Manipulation of quantum information with semiconductor spintronics</i>
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12:00–1:30 Lunch

1:30–2:15	Poul Jessen
	<u>Continuous optical measurement and control of atomic spin ensembles</u>
2:15–3:00	Daniel Lidar
	<u>Concatenated dynamical decoupling</u>

3:00–3:30 Break

3:30–4:15	Gerard Milburn
	<u>Error correction by continuous measurement and feedback</u>
4:15–5:00	Ramon van Handel
	<u>Feedback control of quantum state reduction</u>

5:00–6:30 Discussion, return to hotels

Monday 23 August

8:30–9:30am	Andrew Doherty
	<u>Quantum limits to feedback control</u>

9:30–9:45 Break

9:45–10:45	Howard Wiseman
	<u>Optimal unravelings for feedback control in linear quantum systems</u>

10:45–11:00 Coffee break

11:00–12:00pm	Hans Maassen
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	<u>Quantum filtering and ergodicity of quantum trajectories</u>
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12:00–1:30 Lunch

1:30–2:30	Robert Kosut
	<u>Quantum system identification and detection: design via convex optimization</u>

2:30–2:45 Break

2:45–3:45	Matthew James
	<u>Robustness and risk-sensitive control of quantum systems</u>

3:45–4:15 Break / snacks

4:15–5:15	Andrew Silberfarb
	<u>State tomography by continuous measurement</u>

5:15–5:30 Break

5:30–6:30	Claudio Altafini
	<u>Feedback stabilization of quantum ensembles</u>

Tuesday 24 August

8:30–9:30am	Luc Bouten
	<u>Squeezing-enhanced control</u>

9:30–9:45 Break

9:45–10:45	Jun Zhang
	<u>Geometric control in quantum operation generation</u>

10:45–11:00 Coffee break

11:00–12:00pm	Anthony Bloch
	<u><i>Dynamics and control of coupled oscillator spin systems</i></u>

12:00–1:30 Lunch

1:30–1:50	Axel Andre
	<u><i>Feedback stabilization of atomic clocks using entangled atoms</i></u>
1:50–2:10	JM Geremia
	<u><i>Discriminating between two coherent states</i></u>
2:10–2:30	Daniel Lidar
	<u><i>A Post-Markovian Master Equation</i></u>

2:30–2:45 Break

2:45–3:45	Viacheslav Belavkin
	<u><i>On quantum filtering theory and optimal feedback control</i></u>

3:45–4:15 Break / snacks

4:15–6:30 Workshop caucus

Principles and applications of control in quantum systems

Hideo Mabuchi^{1*} and Navin Khaneja²

¹ *Control and Dynamical Systems, California Institute of Technology*

² *Division of Applied Science, Harvard University*

SUMMARY

We describe in this article some key themes that emerged during a Caltech/AFOSR Workshop on "Principles and Applications of Control in Quantum Systems" (PRACQSYS), which was held 21-24 August 2004 at the California Institute of Technology. This workshop brought together engineers, physicists and applied mathematicians to construct an overview of new challenges that arise when applying constitutive methods of control theory to nanoscale systems whose behavior is manifestly quantum. Its primary conclusions were that the number of experimentally accessible quantum control systems is steadily growing (with a variety of motivating applications), that appropriate formal perspectives enable straightforward application of the essential ideas of classical control to quantum systems, and that quantum control motivates extensive study of model classes that have previously received scant consideration. Copyright © 2004 John Wiley & Sons, Ltd.

KEY WORDS: Quantum, nonlinear, stochastic

1. Introduction

Modern scientific inquiry and the demands of advancing technology are driving theoretical and experimental research towards control of quantum systems. Compelling applications for quantum control have been noted and have motivated seminal studies in such wide-ranging fields as chemistry, metrology, optical networking and computer science. Experience has so far shown that quantum dynamics and stochastics can be incorporated within the framework of estimation and control theory but give rise to unusual models that have not yet been studied in depth. The microscopic nature of quantum systems also demands renewed emphasis on accounting for the essentially physical (finite impedance) nature of measurement and feedback interconnections, which limits the applicability of state-feedback formalism and makes quantum filtering an essential methodology for closed-loop control. Open-loop control remains effective in the quantum regime but the actuation terms are generically bilinear. Overall, one

*Correspondence to: hmauchi@caltech.edu

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begins to see that novel features of quantum systems could spur the growth of a new branch of control theory to develop hand-in-hand with the cutting-edge applications that drive it.

We should be careful to note that theoretical foundations for quantum control have been in place for some time. Among the participants of our small workshop, V. P. Belavkin, H. Rabitz and T.-J. Tarn each reviewed seminal work dating back to the 1980's [1, 2, 3]. But the current resurgence of interest may be attributed to recent advances in experiments on quantum control and to the emergence of high-profile applications in metrology, physical chemistry, quantum information science and spintronics. It thus seems appropriate here to emphasize the importance of grounding further theoretical investigations of quantum control in concrete experimental settings and design goals of practical interest.

Our intent in writing this article is not to present a comprehensive review of the field, but rather to attempt to provide a timely piece—motivated by presentations given at the PRACSYS Workshop—that can indicate some points of entry into the recent literature on quantum control and its applications. We begin with a brief introduction and overview of some compelling applications for quantum control, continue with a survey of relevant experimental systems, and then turn to a more formal presentation of mathematical models and some open problems.

2. Quantum control scenarios and applications

A question that inevitably arises in any introduction of quantum control is, “What makes a control system *quantum*?” In principle, our current understanding of physics holds that all systems are quantum but that manifestly non-classical phenomena are observable only under special laboratory conditions. Roughly speaking, quantum ‘behavior’ emerges in scenarios where a relatively small physical system (with few active dynamical degrees of freedom) can be well isolated from environmental perturbations and dissipative couplings. In some experiments this effectively can be achieved by bringing an experimental apparatus to very low temperatures (as is the case in the superconducting circuit experiments cited below), while in others one can exploit a separation of energy and/or time scales to observe transient quantum behavior at room temperature (as in the experiments performed on atomic ensembles and in liquid-state nuclear magnetic resonance). From a more formal perspective, one could say that quantum mechanics is believed to be a correct microscopic theory of (non-relativistic) physics but that the reduced dynamics of *subsystems* nearly always corresponds closely to models that fall within the domain of classical mechanics. Hence strongly non-classical behavior can only be observed in a subsystem on timescales that are short compared to those that characterize its couplings to its environment. In the case of any macroscopic object, such as an ordinary mechanical pendulum, there are so many such couplings (*e.g.*, via mechanical coupling to its support and to air molecules) that these timescales are inaccessibly short. From an even more abstract perspective, one could say that Schrödinger’s Equation is meant to apply to the universe as a whole (whose ‘internal’ degrees of freedom are densely interconnected) while physical experiments deal only with embedded subsystems. Unless great care is taken to suppress the environmental couplings of an experimental system, the overwhelming tendency is for its behavior to appear classical, or at least imperfectly quantum.

The accurate quantitative modeling of ‘imperfectly quantum’ behavior in open systems (*i.e.*, those with non-negligible residual environmental couplings) is a subject of intense study

in many branches of physics. Generally speaking, one finds fundamental theory in the fields of quantum statistical mechanics and mathematical physics, with more system-specific results in fields such as atomic physics, quantum optics and condensed matter physics. One of the main goals for theoretical research in quantum control will be further to integrate what is known from the physics of open quantum systems with core engineering methodologies.

A second question that may naturally arise at this point is, “*Why* should we study quantum control?” One answer is that the above-mentioned integration of the theory of open quantum systems with estimation and control appears to provide an important new conceptual framework for the interpretation of quantum mechanics itself. By scrutinizing quantum mechanics as a theory for the design of devices and systems, as opposed to a theory for scientific explanation only, we gain new insight into obscure features of quantum theory such as complex probability amplitudes and ‘collapse of the wave function.’ In particular we are able to make more focused comparisons between classical and quantum probability theories. But a second compelling answer to the question at hand is that various branches of research on nanotechnology are advancing to the point of investigating ‘mesoscopic’ devices whose behavior remains quantum on timescales of *functional* relevance. It thus seems clear that in order fully to exploit the powerful methodologies of control theory in the design and implementation of advanced nanoscale technologies, control theory needs to be reconciled with quantum mechanics.

As we hope the following discussion will illustrate, this reconciliation does not appear to require any radical reformulation of control theory. It does however seem that nanoscale systems (broadly defined) and quantum control present new classes of models that fit within the scope of traditional analysis and synthesis methods but have yet to be studied in depth. To date there have been a number of publications that demonstrate the use of standard control-theoretic techniques to analyze models of quantum-physical origin; we will not attempt to review them here. We prefer to emphasize the recent development of concrete applications—tied to experimental research—that generate urgent questions most naturally addressed by quantum extensions of estimation and control theory. These applications and questions are in turn motivating the thorough and principled development of certain practical aspects of quantum control.

A first major application area, to be described in greater detail below, is protein structure determination via nuclear magnetic resonance (NMR). Ideas from control theory have clear relevance to this field because protein structure determination can naturally be viewed as a problem in system identification. In the typical setting one has foreknowledge of the types of atomic nuclei that constitute a given protein, and has experimental tools that can induce rotations of these individual nuclei and collect signals that gauge their precise response to applied controls. The unknown parameters of the system are the relative spatial positions of the various nuclei, which can be inferred from experiment by estimating the relative strengths of the dynamical couplings among them. Questions of optimal procedure arise because measurement signal-to-noise ratios are typically quite low, because dissipative mechanisms suppress the observability of dynamical couplings among the nuclei, and because the total number of measurements that must be made to establish the structure of a protein is tremendously large (thus putting a premium on the speed of the identification procedure). It is intriguing to note that, even though NMR researchers have been working for many decades to optimize relevant techniques, the recent introduction of control theoretic methods has enabled some substantial improvements in performance (with high practical impact). Many further opportunities can

be identified for the application of control theory to NMR.

Over the past decade, a number of groups have proposed and demonstrated close connections between magnetic resonance (of nuclear and/or electronic spins) and quantum information processing. The quantum states of nuclei in certain types of molecules and solid-state systems can be well shielded from environmental perturbations, making them an attractive physical locus for the storage and processing of quantum information. Manipulation of individual nuclear states and conditional transformations of the state of one nucleus based on that of another (corresponding to the implementation of a quantum logic gate) can be accomplished via tailored radio-frequency electromagnetic fields. In this context questions of optimal control arise for much the same reasons as in protein structure determination, with the additional consideration that large-scale quantum computation may require extremely high fidelity (with inaccuracy $\lesssim 10^{-4}$) in these elementary quantum state transformations [4, 5]. This need for high fidelity can be compounded by the fact that in real experiments it is typically necessary (especially in NMR) to work with a sample containing very many identical molecules, in order to make the 'readout' signals sufficiently strong that they can be detected above instrumental noise. The unavoidable presence of inhomogeneities across such a large sample of molecules then demands a certain degree of robustness in the control policies employed, generating further interesting challenges for the theory.

Similar quantum control problems arise in a wide range of physical implementations of quantum information processing. In systems from atomic physics, the nature of the problems is very similar to what has been described above for the setting of magnetic resonance. In solid-state systems, one generally finds an intriguing combination of issues of both identification and control. Whereas accurate *ab initio* models can often be constructed for NMR and atomic systems, the modeling of solid state systems typically requires a more phenomenological approach. In particular, it is seldom possible to derive accurate models for the residual environmental couplings of something like a superconducting quantum circuit. The precise nature and strength of these couplings should be known in order to design control schemes that maximize the fidelity of elementary quantum operations, which as discussed above should be very close to perfect if one is ultimately interested in large-scale quantum computation. Some recent theoretical research [6, 7, 8] has also shown that tools from control and dynamical systems theory can play a substantial role in the formulation and analysis of fault-tolerant architectures for quantum computation and communication.

Quantum computation represents a very high-profile long term goal in nanoscale science and technology; the related field of *quantum metrology* (or quantum precision measurement) provides a setting with similar technical challenges and with near-term payoffs for the exploitation of quantum control. In applications of high strategic and industrial interest, such as prompt and accurate estimation of magnetic fields, electrical currents, time delays, gravitational gradients, accelerations and rotations, it is just now becoming possible to construct laboratory prototype systems whose leading-edge performance is enabled by techniques that exploit quantum coherence and is limited by noises or uncertainties of quantum-mechanical origin. In these contexts it is natural to look to quantum control to provide techniques for achieving robust performance, based on approaches such as optimal design, adaptation and real-time feedback. Preliminary studies grounded in several different experimental settings [9, 10] have shown, *e.g.*, that real-time feedback can be used to preserve quantum-limited sensitivity gains in the presence of multiplicative uncertainties that would otherwise nullify them. Concrete targets for the application of such methodology range from

atom interferometer-based inertial sensing systems to grand scientific projects such as the Laser Interferometer Gravitational Wave Observatory (LIGO). In both of these examples [11, 12, 13], promising strategies exploiting quantum phenomena have been formulated to surpass near-term performance limits, but quantum control techniques will likely be required in order to implement them robustly.

The final application area we wish to highlight is control and identification of chemical reactions. As has been discussed in some excellent recent review articles [14, 15], tailored laser pulses can be used to induce and to steer molecular processes ranging from fragmentation [16] to electron transfer [17] and high-harmonic generation [18]. It has been noted that the typically complex nature of the interaction between applied fields and intrinsic dynamics in an optimal control solution could make it possible to design highly selective and sensitive approaches to detecting dangerous chemicals in an environmental monitoring scenario [19, 20]. An interesting feature of recent work on control of chemical reactions is that highly successful control solutions have been 'discovered' using learning loops that combine computer optimization algorithms with fast and automated laboratory apparatus for *experimentally* (as opposed to computationally) evaluating the performance of trial solutions. Such an approach is particularly powerful in the chemical reaction setting as it is often infeasible to obtain accurate models for the relevant molecular dynamics. Early experimental successes have provided strong motivation for theoretical research on improved learning algorithms and on methods for 'inverting' the empirically-optimized control solutions to infer pertinent properties of the molecular dynamics.

In the applications described in this paper, some common themes and problems emerge from the standpoint of mathematical control theory. Many experiments and applications involving control of quantum dynamics like magnetic resonance involve manipulation of quantum ensembles. The members of the ensemble though having identical dynamics, could show a big dispersion in their physical parameters that characterize the dynamics. The control challenge is to find excitations that are robust to these dispersions and inhomogeneities. These problems lead naturally to study of a class of infinite dimensional systems that are highly under-actuated, as one is trying to steer a continuum of systems using the same control. Such control models raise interesting issues of controllability that are discussed in Sec. 4.3. Besides questions related to controllability of finite and infinite quantum systems, there are a class of optimal control problems that arise naturally in coherent control of quantum phenomenon. Since most quantum systems in practice are open, excitations that steer quantum systems between states of interest in minimum time are desirable, as they reduce dissipative effects of environment. From perspective of mathematical control theory, many of these problems reduce to time optimal control of bilinear systems evolving on finite or infinite dimensional Lie groups. Although, bilinear control problems have been studied in great detail in classical control literature, rich mathematical structures dictated by new physical problems arise. In many cases, the added structure leads to complete characterization of time optimal trajectories and reachable sets for many of these systems [21, 22]. These results of fundamental and practical interest in the areas of spectroscopy and quantum information are described in some detail, in Sec. 4.1. Another class of optimal control problems that are ubiquitous in applications of quantum control is steering of quantum mechanical systems in presence of relaxation. The control challenge is to characterize the reachable set of dissipative bilinear control systems and corresponding optimal controls. Recent work has shown that by systematic use of methods of optimal control, significant improvement can be made in sensitivity of multidimensional NMR

experiments [23, 24, 25]. The study of these open quantum systems leads naturally to a new class of constrained bilinear systems. These problems are discussed in Sec. 4.2. We believe, the new mathematical structures that arise in problems of manipulation of quantum dynamics are excellent motivation for further developments in control theory.

The problems in closed loop control described are also a rich source of new problems in estimation, filtering and feedback control. Building on seminal work in quantum probability and quantum filtering theory, it has been possible to derive exact results for 'quantum LQG' problems that correspond very closely to analogous results in classical Linear Quadratic Gaussian control. It has also been established that general problems in quantum feedback control can be approached via a separation principle, such that all of the uniquely quantum-mechanical considerations are subsumed in the derivation of appropriate filtering equations [26]. Control synthesis can then be viewed as a problem of state feedback on the estimator. The availability of quantum filtering equations also enables rigorous approaches to (open- and closed-loop) quantum parameter estimation and quantum system identification. In addition to the intrinsic interest of these subjects, we should note that they represent very important problems within fields such as quantum information science and quantum metrology.

3. Experimental systems

In this section we provide brief overviews of three broad classes of experimental systems with close ties to quantum control. As mentioned above, coherent control of molecular dynamics and chemical reactions has recently been reviewed [14, 15] by experts in the field, so we will refer the interested reader rather than synopsizing their materials here. While tutorial introductions are beyond the scope of this article, our aim is to provide theoretical and experimental references in a manner that highlights points of interest to the controls community.

3.1. Magnetic resonance

Few analytical techniques in science match in the breadth and depth the impact achieved by nuclear magnetic resonance (NMR). Starting as a tool for characterization of organic molecules, the use of NMR has spread to areas as diverse as pharmaceuticals, metabolic studies, structural biology, solid state chemistry, condensed matter physics, rheology, medical diagnostics (medical resonance imaging) and more recently neurobiology [27, 28, 29]. The principles of NMR have served as paradigm for other physical methods that rely on interaction between radiation and matter. It is therefore not surprising that experiments in NMR also serve as good model problems in control of quantum systems. In this section, we present a quick review of the basics of magnetic resonance for understanding control problems arising in various multidimensional experiments in high resolution NMR spectroscopy.

Modern NMR experiments, use a large static magnetic field B_0 (say pointing in the z direction) of the order of 5-20 Tesla to align magnetic moments of atomic nuclei in a sample along its direction. The resulting net magnetization \vec{M} in the direction of B_0 is then manipulated by an oscillating radio frequency field $(B_x(t), B_y(t))$ in the $x - y$ plane, which is smaller than B_0 by 4 to 5 orders in magnitude. This field exerts a torque on \vec{M} , which then

evolves as a bilinear control system

$$\frac{d}{dt} \begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix} = \gamma \begin{bmatrix} 0 & -B_0 & B_y(t) \\ B_0 & 0 & -B_x(t) \\ -B_y(t) & B_x(t) & 0 \end{bmatrix} \begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix}. \quad (1)$$

An oscillating $(B_x(t), B_y(t))$ at the Larmor frequency $\omega_0 = \gamma B_0$, (γ is the gyromagnetic ratio of nuclei) i.e. $(B_x(t), B_y(t)) = (A \cos(\omega t), A \sin(\omega t))$, transfers the magnetic moment vector $\vec{M}(0) = (0, 0, 1)$, to the $x - y$ plane. At this point, the oscillating field is switched off and the magnetic moment precesses around the static magnetic field B_0 with a frequency ω_0 . This precessing magnetic moment induces a current in a nearby coil also termed as free induction decay (FID). This FID, when fourier transformed, shows a peak at ω_0 , a characteristic of the nuclei. At a field of 14 Tesla, the Larmor frequency of proton (^1H), nitrogen (^{15}N) and carbon (^{13}C) is 600 MHz, 60MHz and 150 MHz respectively. NMR is therefore an important analytical tool in chemistry as the peaks in the spectra reveal the chemical composition of molecules. The magnetic moments making the magnetization vector \vec{M} experience local fluctuations in the ambient field B_0 causing them to loose coherence (decoherence). This gives the FID, an decaying envelop and the peaks in the spectrum their line widths (see Fig. 3.1).

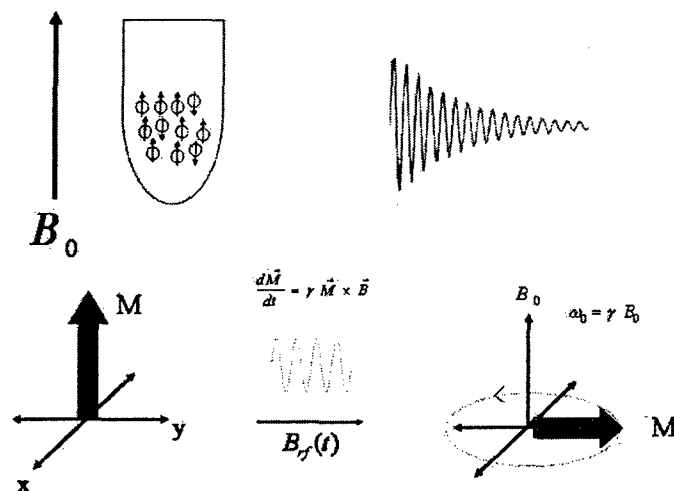


Figure 1. The figure shows the basic features of an NMR experiment. The top left of part of the figure depicts use of a field B_0 to polarize the sample. The bottom figure shows use of pulsed magnetic fields to steer the net magnetization and generate FID. The top left panel shows the profile of a free induction decay.

The experiments in structure determination of biomolecules using NMR [30, 31] begins with collecting a proton spectra. Protons in the molecule have different electronic environments. These electronic currents generate small magnetic fields which alter the static field B_0 locally, hence shifting the Larmor frequency of these protons. The resulting proton spectrum has many peaks as depicted Fig. 3.1 A. These shifts in the Larmor frequency are characteristic of the

chemical environment of the spins. Based on these chemical shifts, it is possible to assign the various peaks in the spectrum of a molecule to various protons, a process called frequency labeling [30]. Following this, a series of experiments are used to study interaction between various frequency labeled protons, which gives information on distance between protons of various amino acids. This information is used to solve for a folded configuration that satisfies these distance constraints. In practice, the proton spectrum of a large protein molecule is poorly resolved as shown in Fig. 3.1 B. This is due to crowding of the spectrum by larger number of proton resonances and their increased line widths caused by increased decoherence rates of larger proteins.

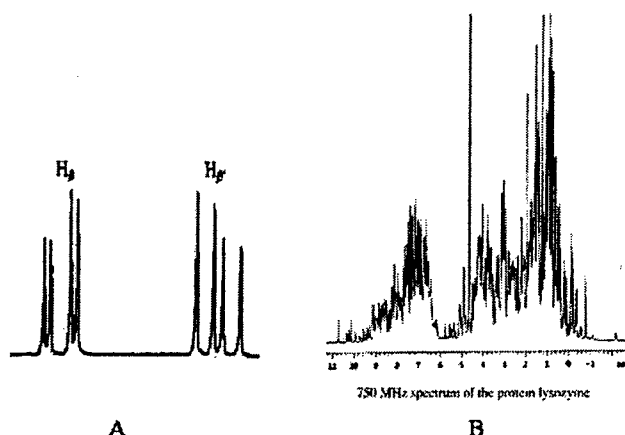


Figure 2. Panel A shows the proton spectrum of a small peptide. The proton resonances are clearly resolved. Panel B shows the proton spectrum of protein Lysozyme at a magnetic field corresponding to proton frequency of 750 MHz. The spectra has overlapping resonance lines.

To circumvent this problem, methods of multidimensional NMR were invented [27]. The multidimensional NMR experiments generate a two dimensional spectrum, where each peak in the spectrum is labeled by Larmor frequencies of a coupled spin pair. For example, the first label could be the Larmor frequency of a proton and the second label the Larmor frequency of another spin coupled to proton, say ^{15}N . As a result, the two protons, with overlapping Larmor frequencies can now be distinguished by their nitrogen frequencies. This way, the one dimensional spectrum of protons can be resolved and peaks assigned a unique frequency label. The basic set up of two dimensional NMR experiment is depicted in Figure 3.1. Initially spins S are excited by an oscillating magnetic field with frequency corresponding to approximately their Larmor frequencies. The net magnetization of the spins S is driven to transverse plane where it precesses for some time t_1 . Then by application of external rf field and the coupling between the spins the magnetization is transferred from spin S to spin I . The spins I are then excited and the precession of its magnetization is recorded. The experiment is performed again by incrementing the value of t_1 , resulting in a two dimensional signal $s(t_1, t_2)$ indexed

by the time t_1 of the precession of the spin S and t_2 , the time of the precession of spin I . This signal takes the form $s(t_1, t_2) = \eta \cos(\omega_S t_1) \cos(\omega_I t_2) \exp(-R_S t_1) \exp(-R_I t_2)$, where R_I and R_S are relaxation rates for spin I and S respectively and η is the efficiency of the magnetization transfer step. A two dimensional fourier transform of this signal gives peak at frequency (ω_I, ω_S) . The relaxation rates R_I and R_S determine the linewidths and η , governs the sensitivity of the experiment.

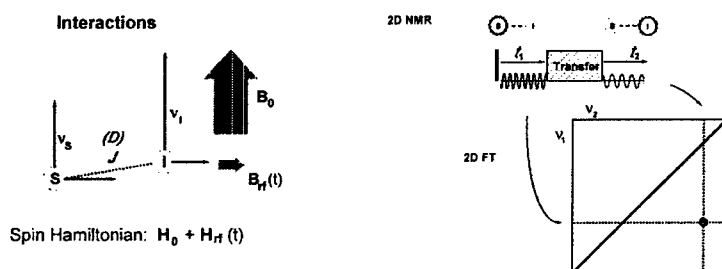


Figure 3. The left panel shows a coupled two spin system where interactions are used to transfer magnetization between coupled spins. The right panel shows the basic features of a 2-dimensional NMR experiment where magnetization on spin S evolves for time t_1 followed by a transfer to spin I and then another evolution period t_2 .

The basic idea of a 2D NMR experiment can be extended to 3 or 4 dimensional experiments which generates frequency information of spins in a coupled spin network. In NMR spectroscopy of proteins, many such elaborate experiments have been developed to improve resolution of the data [31]. There are numerous, beautiful control challenges, related to finding the optimal rf-excitations that optimize the efficiency of transfer of magnetization in a network of coupled spins. From perspective of control theory, these are control problems related to steering bilinear control systems with drift. Finding the shortest time optimal pulse sequences, that transfer magnetization between coupled spins or minimize relaxation losses and thereby maximize η has been a long standing research area in NMR spectroscopy. Only recently have these problems been addressed from a control theory perspective. These problems involve computing reachable sets of bilinear control systems with drift. Physics imposes new mathematical structures in these problems. This has made it possible to characterize optimal trajectories of these bilinear control systems [21, 22, 23, 24, 25]. There are numerous open problems that can benefit from systematic application of tools from control theory. These problems of optimal control of coupled spin topologies have a direct bearing on the area of quantum information. Finding optimal excitations to generate a desired evolution in a network of coupled quantum systems is a canonical problem in area of quantum information. These problems are discussed in some detail in Sec. 4.1-4.3.

3.2. Atomic physics

Basic studies of atomic internal degrees of freedom (which determine their characteristic absorption and emission spectra) were crucial for the early development of quantum mechanics, and in recent years atomic systems have again become the focus of seminal research in quantum control and related fields. Because of their relative simplicity and the ease with which they can be well isolated from bulk matter, gas-phase atoms provide a canonical setting in which to validate elementary methodology. Subtle techniques have already been developed for the manipulation of electron orbital motion and hyperfine spin dynamics, with potential applications in quantum information processing and metrology. The invention and refinement of laser cooling techniques have made it possible to observe and to induce quantum phenomena in the center-of-mass motion of atoms as well; various forms of matter-wave interferometry are now widely studied and there has recently been an explosion of activity in the study of quantum phase transitions of cold atoms in optical lattices.

Quantum control techniques that have previously been developed by the atomic physics community are mainly of intuitive origin. In many cases they were adapted from earlier work in magnetic resonance [28, 29]. But researchers working on atomic systems have begun to explore the utility of robust pulse sequences from NMR [33] and of optimal control theory [32] as it has been formulated by physical chemists [2], and have likewise succeeded in generalizing some principles from elementary frequency domain feedback control [34, 35] (a working knowledge of which is required for the design and maintenance of most atomic physics experiments). As it is often possible to model atomic systems essentially from first principles, sophisticated synthesis techniques from control theory may prove to have great practical utility and to enable vastly improved performance. Preliminary investigations suggest that model complexity can be a serious obstacle, however, as can limitations on current technical capabilities for generating complex laser control fields. Atomic dynamical timescales can also be quite short (lying generally in the range from $\sim 10^{-9}$ to $\sim 10^{-3}$ seconds), which presents a challenge for the implementation of closed-loop methods. Rigorous model reduction, robustness and 'non-fragility' will thus be highly desirable in the development of quantum control for atomic systems.

It is important to note that there is a solid theoretical foundation for the physical modeling of input and output channels for atomic control systems. In particular, continuous measurements based on the scattering of laser light by atoms can be accurately modeled, thus enabling a rigorous treatment of the quantum mechanical measurement 'backaction' in quantum feedback control (see Sec. 4.4).

Several distinct classes of atomic experimental systems can be identified with relevance to quantum control. After decades of intense laboratory development, trapped ions now provide a very clean realization of the elementary quantum model of one or more spins coupled to simple harmonic oscillators. Relatively long coherence times can be obtained in trapped ion experiments together with very low effective temperatures; they have thus become quite important for applications in frequency metrology [36] and quantum information processing [37]. Various techniques have been established for manipulating the quantum state of trapped ions via lasers and electric fields, and some of these have been analyzed from the perspective of geometric control theory [38, 39]. As far as open-loop control is concerned, trapped ions have provided some of the most sophisticated examples of quantum control to date. One potential drawback of these systems (for fundamental studies in quantum control) is that real-time

monitoring of dynamical variables in a small sample of trapped ions is extremely difficult if not impracticable (see, however [40, 41] for significant recent progress). For practical applications this could be less of an impediment than a control engineer might imagine, however, as stochastic perturbations can be kept relatively small in these experiments, high purity (low entropy) initial states can be prepared, and many useful quantum states are reachable with current actuation capabilities.

Many of the attractive features of trapped ions, such as relatively long coherence times and the reachability of highly non-classical states, can also be found in single-atom cavity quantum electrodynamics (cavity QED) [42]. In modern cavity QED, the specially-arranged environment of an electromagnetic resonator with high quality factor and small mode volume is utilized to achieve strong coupling between individual atoms and photons. Experiments conducted in the microwave regime [43, 44], with Rydberg atoms and superconducting resonators housed in a cryostat, have achieved quantum control results on par with what has been accomplished using trapped ions. Experiments in the optical regime [45], with ground-state atoms and dielectric mirror resonators, have recently begun to produce ground-breaking results in active control of quantum dynamics as well [46] (with potential applications in quantum communication and cryptography). For the current discussion, optical cavity QED has the significant additional feature of being the one of the few experimental settings in which it is currently possible to perform continuous measurement of quantum dynamical variables, as would be required for real-time feedback control. Several theoretical papers can already be found that investigate applications of filtering and feedback in cavity QED, *e.g.*, for active cooling of the motion of a single atom [47] or for control of the atomic resonance fluorescence spectrum [48]. Early interest in aspects of quantum control for cavity QED was stimulated by potential applications in quantum information science, and also by a strong general interest within the field in non-equilibrium statistical mechanics and the quantum-classical interface [49].

Experiments on large ensembles of atoms have also recently entered the domain of quantum control. Here one sub-class of experiments utilizes simple vapor cell samples, in which special technical preparations can be used to enable long coherence times for collective internal quantum degrees of freedom of gas-phase atoms whose center-of-mass motions are at equilibrium at room temperature. Both open-loop [50] and closed-loop [51] experiments have been conducted with significant interest to quantum control, although the direct motivation of these works was more along the lines of quantum information science. A second sub-class of experiments on atomic ensembles works with laser-cooled clouds of gas-phase atoms. Again, both open- [52, 53] and closed-loop [54] experiments have been performed, with motivations stemming from both metrology and quantum information science. The open-loop work on interfering pathways in laser excitation of electronic orbital motion provides a compelling demonstration of a key principle from the physical chemists' perspective on quantum control, and may have the potential to find practical application in stability transfer of optical frequency standards [55]. The closed-loop work is related both to feedback stabilized preparation of quantum states (for fundamental studies or for quantum information applications) and to proposed schemes [10] for robust atomic magnetometry (magnetic field measurement). The latter work connects current experiments to more formal theoretical work on linear quadratic Gaussian (LQG) quantum control, quantum filtering and quantum parameter estimation (see Sec. 4.4 and Sec. 4.5 below).

Although the essential ideas involved in quantum control with atomic ensembles are similar to those of NMR, we should emphasize that the atomic experiments manipulate pure (or nearly

pure) quantum states whereas the liquid-state NMR research described above generally works with so-called effective pure states [56]. Magnetic resonance experiments with low temperature solid-state samples [57] or electron spins [58] are more like atomic systems in this regard.

Finally, we wish to call attention to a new class of experiments on atoms in optical lattices. Optical lattices are one-, two- or three-dimensionally 'corrugated' mechanical potentials, created by laser light, that can be used to modulate the motion of cold atoms and even confine them in crystalline arrays. The interaction between the laser light and the atomic center-of-mass motion depends generally on the atomic internal state, which makes optical lattices an interesting setting in which to couple these quantized degrees of freedom [59] (much as has been done with trapped ions). Experiments have been proposed to investigate the crossover from chaotic classical dynamics to quantum dynamics in such systems [60], and also to implement quantum logic gates among neighboring atoms in the lattice [61, 62, 63, 32]. When an optical lattice is 'loaded' from a degenerate quantum gas, such as an atomic Bose-Einstein condensate, it is possible to observe intriguing quantum phase transitions of the kind that have long been studied in condensed matter physics [64, 65]. Theoretical studies have begun to appear on the possibility of actively controlling these quantum phase transitions in order to access exotic atomic collective states [66, 67].

3.3. Solid-state systems

Solid-state systems provide very rich dynamical settings for the investigation of quantum phenomena. The construction of accurate theoretical models for such systems can be quite challenging, but it has been possible to achieve excellent agreement with experiments in numerous scenarios of interest for quantum control. Here we will limit our attention to a brief survey of some specific systems that were discussed at the PRACQSYS workshop, with a selection of compatible experimental and theoretical references. As a general comment, it seems worthwhile to note that recent work on quantum control of solid state systems strongly suggests that some practical limits to achievable performance will derive from the finite temperature of sensors and actuators; this is an unusual and interesting 'physical' consideration for estimation and control.

Superconducting circuits incorporating Cooper-pair boxes have become a central paradigm for the study of many-body quantum dynamics, mesoscopic physics and solid-state realizations of quantum information processing. It is now possible to produce coherent superpositions of quantum states of such circuits, to observe coherent dynamical evolution in them, and to perform readout with high fidelity and low backaction [68]. Open-loop quantum control in superconducting circuits is thus reaching a level of maturity comparable to that of trapped ion systems, although the decoherence mechanisms (residual environmental couplings) are much less well understood and the achieved control fidelities have accordingly been substantially lower. However, superconducting circuits provide access to a broader range of dynamical phenomena, including bifurcations and limit-cycle behavior for quantized effective degrees of freedom; some of these have been well characterized and even exploited as the basis for constructing novel quantum amplifiers [69]. Recently it has become possible to couple Cooper-pair boxes to high quality factor microwave resonators [70], leading to the realization of 'circuit QED' systems with many features in common with single-atom cavity QED as described above. These developments have opened exciting new prospects for observing conditional evolution and possibly implementing real-time feedback control in superconducting circuits.

Electron spin degrees of freedom in semiconductor systems can likewise serve as subjects for quantum control, with important practical applications in the emerging information technology paradigm of 'spintronics.' Here the vision is to utilize electron spin (rather than charge) as the carrier of information in computer circuitry, with concomitant potential gains in speed and miniaturization. One possible drawback to the use of electron spins is the relative difficulty of implementing control mechanisms to change their states rapidly and with high spatial selectivity. By analogy with NMR experiments, for example, one would think of using pulsed magnetic fields to manipulate spins but this would be very difficult to do with the required speeds and localization. But it has recently been demonstrated that one can instead utilize the effective magnetic fields (due to the relativistic transformation of local electric fields) seen by electrons moving at high speed through a strained semiconductor [71]. This insight could provide the basis for crucial further developments, with numerous opportunities for control theoretic analysis and design. These relativistic effects create an unusual dynamical coupling of an electron's spin (intrinsic angular momentum) to its linear velocity, which should be quite interesting to study from the perspective, *e.g.*, of geometric control.

One final development we wish to mention is the impressive recent progress on reaching a quantum regime for the dynamics of nano-scale *mechanical* oscillators [72, 73]. Here the fabrication of sub-micron scale cantilevers with extremely low internal dissipation and weak environmental couplings, combined with state-of-the-art cryogenics and cryogenic electro-mechanical sensors, has made it possible to approach conditions in which quantum-mechanical behavior of the cantilever should become observable and controllable. Initial theoretical studies have been conducted of the feasibility of using real-time feedback for active cooling of a cantilever to its quantum mechanical ground state [74], and strategies have been proposed and analyzed [75] for coupling a nano-mechanical cantilever to a Cooper-pair box to provide an alternative solid-state realization of dynamics analogous to that of single-atom cavity QED.

4. Models and problems arising in quantum control

The applications and experimental systems described above have given rise to many theoretical research challenges in quantum control. Here we discuss a selection of them and provide references to relevant publications.

4.1. Bilinear and Geometric control problems in Quantum systems

Active control of quantum dynamics involves systematically changing the Hamiltonian of the quantum system by suitably tailored electromagnetic fields. These are bilinear control problems (usually with drift) involving control of the unitary evolution operator U evolving under Schrödinger equation ($\hbar = 1$)

$$\dot{U} = -i[H_d + \sum_{j=1}^m u_j H_j]U. \quad (2)$$

H_d is the internal Hamiltonian of the system representing couplings between various degrees of freedom and H_j are the Hamiltonians resulting from external excitations which are modulated using choice of control $u_j(t)$. There has been significant interest in understanding the controllability properties of these systems [83, 99, 100, 101, 102, 103, 104], both when the

quantum system (and hence U) is finite dimensional, as in architectures of coupled spins and in cases where U is infinite, as arising in problems ranging from control of cold trapped ions to control of molecular reactions using laser fields [38, 39, 103].

In the finite dimensional case, results on controllability of these systems are well known from classical control theory [91, 92, 93] and captured by the Lie algebra $\{-iH_d, -iH_j\}_{LA}$ generated by the Hamiltonians H_d and H_i . In the case of infinite-dimensional bilinear control systems, many conceptual and technical difficulties remain [38, 39]. Controllability arguments for steering infinite dimensional systems, between eigenstates of interest have been primarily constructive [96, 97]. There has been a recent interest in understanding controllability of infinite dimensional quantum systems from perspective of geometric control theory, though much work remains to be done. Infinite dimensional bilinear control problems also arise naturally in the context where one is trying to steer an ensemble of finite dimensional quantum systems [87, 88, 89, 90]. These problems are discussed in much more detail in the following section 4.3.

Besides questions of controllability, in practice, the complexity of synthesizing excitations, that produce a desired evolution of a quantum system is of great interest. In general, external excitations, must cooperate with evolution under the intrinsic Hamiltonian H_d to synthesize a desired evolution such as transferring coherence between spins in context of magnetic resonance, creation of entangled states or synthesis of quantum logic between coupled quantum systems [21]. This reliance on internal evolution puts a fundamental limit on the amount of time it takes to implement a desired unitary evolution in a quantum system. This is a known fact in control theory. For controllable nonlinear systems with drift, there is in general a minimum time to steer the system to a desired point even in the presence of unbounded controls. Characterizing all unitary transformations that can be synthesized in a given time is an important problem related to the design of time-optimal excitations for bilinear control systems with drift [21, 22]. The problems are of practical importance, as quantum systems of interest are rarely isolated from their environment. Finding time optimal methods to steer the system in Eq. 2 between points of interest reduce dissipative effects caused by interaction with the environment.

Recent study of these time-optimal control problems has led to a careful study of the relationship between Lie algebras generated by control Hamiltonians $\mathfrak{k} = \{-iH_j\}_{LA}$ and the full control algebra $\mathfrak{g} = \{-iH_d, -iH_j\}_{LA}$ and the associated groups $K = \exp(\mathfrak{k})$ and $G = \exp(\mathfrak{g})$ [21]. The time required to synthesize a desired evolution in Eq. 2 can be related to control systems on the quotient space G/K . A satisfactory theory has emerged when the quotient space G/K is a Riemannian symmetric space [21]. These spaces arise naturally in the study of control of coupled spin $\frac{1}{2}$ [21, 22, 98] in context of magnetic resonance and quantum information processing. In this case, the space G of unitary transformation of coupled spins is $SU(4)$. The external excitations produce local unitary transformations in the subgroup $K = SU(2) \otimes SU(2)$. Analysis of the resulting control systems on the symmetric space $\frac{SU(4)}{SU(2) \otimes SU(2)}$ [21, 98, 108] has made the synthesis of unitary transformations for coupled spin $\frac{1}{2}$ or qubits transparent. The associated Cartan decomposition of $SU(4)$ in terms of the subgroup $SU(2) \otimes SU(2)$ has been used extensively for design of quantum gates in quantum information sciences [83, 98, 109, 110, 111, 112]. Many of the entanglement generation properties of the quantum gates can be studied using these Cartan decompositions [112]. The reachable sets and time optimal controls in Eq. 2 can be completely characterized when G/K is a Riemannian symmetric space [21]. Many of these time optimal control designs have been experimentally

realized in the context of magnetic resonance [80, 81].

The geometric control methods hold promise for understanding problems of optimal control design in more elaborate scenarios involving networks of coupled quantum systems in various quantum information processing architectures. Many of these optimal control problems reduce to the study of subriemannian geodesics [94] on homogeneous spaces [22]. In the general problem of control of a network of coupled spin $\frac{1}{2}$, the control subgroup $K = SU(2) \otimes SU(2) \otimes \dots SU(2)$ of local unitary transformations, is much smaller compared to the group of all the unitary transformations $G = SU(2^n)$. Finding efficient ways to realize unitary evolutions in a network of coupled quantum systems are interesting challenges in the geometric control of practical relevance. For infinite dimensional quantum systems, the problems of optimal control design are mainly open [39]. Besides generation of specified unitary evolutions, there are important time optimal control problems related to state to state transfer. These range from problems of optimal synthesis of entanglement and transfer between eigenstates in a chain of trapped ions [38] to transfer of polarization along a spin chain [79].

Although study of bilinear control systems is not a new subject, new physical problems arising in control of quantum systems motivate rich mathematical structures. These problems therefore provide further motivation for development of nonlinear and geometric control theory.

4.2. Optimal Control of Quantum Dynamics in the Presence of Relaxation

In practice, the interaction of a quantum system with its environment makes the evolution non-unitary and relaxes the system back to its equilibrium state. This in various applications leads to loss of signal and information. This problem of relaxation is ubiquitous in applications involving coherent control of quantum mechanical phenomenon. Manipulating quantum systems in a manner that minimizes relaxation losses is a fundamental challenge of practical importance.

In recent years there has been significant interest in the development of the techniques for optimal control of quantum dynamics in presence of relaxation, primarily in the context of magnetic resonance [23, 24, 25, 85, 86]. Most of the work in this area has focused on applications, where the environment can be approximated as an infinite thermostat and the evolution of the open quantum system can be modeled by an equation of the Lindblad type [77, 78]

$$\dot{\rho} = -i[H_d + \sum_j u_j(t)H_j(t), \rho] + L(\rho). \quad (3)$$

The evolution of the state of the quantum system is no longer unitary, but the control system still retains its bilinear structure as the term $\rho \rightarrow L(\rho)$ is a trace preserving linear mapping.

From the standpoint of control theory, these are interesting challenges related to the control of the Lindblad equation. How close can the state of a quantum system be driven to its target state? What is the maximum sensitivity one can expect in an multidimensional NMR experiment, or what is the maximum entanglement that can be synthesized in an open quantum system. All these questions are directly related to computing the reachable sets of Lindblad equations. In high resolution NMR experiments significant improvement in sensitivity has been reported for various experiments [25, 23, 24, 85, 86] by optimal control of the systems as in

Eq. 3. There has also been some recent work on understanding the controllability properties of these systems [105] from a mathematical control theory perspective.

To fix ideas, we present a model problem associated with optimal control of coupled spin dynamics in the presence of relaxation [24]. Given the control system [82]

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 & -u & 0 & 0 \\ u & -k & -J & 0 \\ 0 & J & -k & -v \\ 0 & 0 & v & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \quad (4)$$

with $k, J > 0$, the objective is to find out that starting with the state $(1, 0, 0, 0)$, what is the maximum achievable value of x_4 and what are the optimal controls u and v that achieve this value. Observe, even if the strength of controls is unbounded, there is a fundamental limit on the maximum value of x_4 .

The study of optimal control of systems of the above kind leads to new class of constrained bilinear control systems where the control parameters can be expressed as polynomial functions of fewer parameters [24, 82]. For example, consider the optimal control problem of finding the largest value of r_2 that can be reached for the system

$$\frac{d}{dt} \begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix} = \begin{bmatrix} -ku_1^2 & -Ju_1u_2 \\ Ju_1u_2 & -ku_2^2 \end{bmatrix} \begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix} \quad (5)$$

starting with $(r_1(0), r_2(0)) = (1, 0)$, where controls $-1 \leq u_i \leq 1$. Observe the controls u_1 and u_2 enter quadratically in the above equation 5, which helps us to analytically solve for the optimal control [24].

In general, these problems on control of open quantum systems then motivate the study of constraint bilinear control problems, of the following form. Let $x \in \mathbb{R}^n$ and $u \in \mathbb{R}^m$. Consider the system

$$\dot{x} = (A + \sum_i f_i(u) B_i) x, \quad (6)$$

where $f_i(u)$ is a polynomial or more general function of control parameters u . Find the reachable set of such a system starting from some initial state x_0 . Problems of optimal control of Lindblad equations also arise naturally in the context of laser cooling. Recently, these control problems have been studied with the goal of finding optimal excitations to minimize the entropy of a quantum system [106, 107].

A systematic study of the controllability and optimal control problems related to Lindblad equations of open quantum systems is expected to have immediate impact in areas of coherent spectroscopy and quantum information processing.

4.3. Control of ensembles

Many applications in control of quantum systems involve controlling a large ensemble by application of the same control. In practice, the elements of the ensemble could show variation in their physical parameters that govern the dynamics of the system. For example, in magnetic resonance experiments, the spins of an ensemble may have large dispersion in their Larmor frequencies, strength of couplings between coupled spin pairs and the relaxation rates of the spins. In solid state NMR spectroscopy of powders, the random distribution of orientations

of inter-nuclear vectors of coupled spins within an ensemble lead to a distribution of coupling strengths [76]. A canonical problem in control of quantum ensembles is to develop external excitations that can simultaneously steer the ensemble of systems with variation in their internal parameters from an initial state to a desired final state [87, 88, 89, 90]. From the standpoint of mathematical control, the challenge is to simultaneously control a continuum of systems between points of interest with the same control, for example transfer of magnetization in coupled spin ensemble with large variations in the Larmor frequencies and coupling strengths.

To fix ideas, consider the following bilinear control system that captures the dynamics of an ensemble of spin $\frac{1}{2}$ in external magnetic field as described in section 3.1.

$$\frac{d}{dt} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 & -\omega & -au(t) \\ \omega & 0 & av(t) \\ au(t) & -av(t) & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \quad (7)$$

Consider now the problem of designing controls $u(t)$ and $v(t)$ that simultaneously steers an ensemble of such systems with their natural frequency $\omega \in [-B, B]$ from an initial state $(x, y, z) = (0, 0, 1)$ to a final state $(x, y, z) = (1, 0, 0)$ [87]. This problem is of particular interest, when the maximum amplitude of the applied field $A(t) = \sqrt{u^2(t) + v^2(t)}$ is comparable to or less than the bandwidth B one is trying to cover [87].

These problems raise interesting questions about controllability, i.e showing that there exists a control law $(u(t), v(t))$ satisfying $\sqrt{u^2(t) + v^2(t)} \leq A_{max}$ which simultaneously steers all the systems with $\omega \in [-B, B]$ to a ball of chosen radius around the final state $(1, 0, 0)$ in finite time. Furthermore, practical considerations like relaxation as described in section 3.1, make it desirable to construct the shortest control law which achieves this goal. These are problems of optimal control of infinite dimensional systems of a special kind. A systematic study of these systems is expected to have immediate applications in areas of coherent spectroscopy and control of quantum systems in general. Generalization of these problems to controllability and optimal control questions related to the problem of transferring an initial function $(x(\omega, 0), y(\omega, 0), z(\omega, 0))$ to a target function $(x(\omega, T), y(\omega, T), z(\omega, T))$ by an appropriate choice of controls in Eq. 7 is particularly interesting and relevant in NMR and MRI applications. In this context, Eq. 7 can be interpreted as a partial differential equation, where the functions $x(\cdot, \cdot)$, $y(\cdot, \cdot)$ and $z(\cdot, \cdot)$ have both a dependence on time t and the parameter ω . Therefore these problems motivate investigating the controllability properties of bilinear PDE models of the form

$$\frac{dx(s, t)}{dt} = (A(s) + \sum_i u_i(t) B_i(s)) x(s, t)$$

where the same controls $u_i(t)$ are being used to simultaneously steer an ensemble of control systems indexed by the control parameter s . These models include problems in which the elements of an ensemble may see a big variation in the control field. In Eq. 7, the parameter a might show a distribution in $a \in [A_{min}, A_{max}]$. In magnetic resonance applications, this arises when different spatial positions in the sample experience different rf-fields due to field inhomogeneities. Control designs that only excite parts of the ensemble with their parameter values in a desired region and leave the remaining ensemble undisturbed are desirable in NMR and MRI applications [95].

Another class of problems that arise often in the control of quantum ensembles are the ones associated with the optimization of certain average quantity associated with the ensemble. To fix ideas again consider the model problem of optimal state transfer in the presence of relaxation described in Eq. 4 in section 4.2 [24]. Now J and k are distributed in the range (J_1, J_2) and (k_1, k_2) respectively. The goal is to design $u(t)$ and $v(t)$ that maximize the average value of x_4 over all the systems i.e maximize

$$\int_{J_1}^{J_2} \int_{k_1}^{k_2} x_4(J, k, t) dJ dk.$$

In summary, problems involving simultaneous control of a continuum of systems with dispersion in their parameters arise naturally in control of quantum ensembles. These problems have received little in-depth attention in the past in control theory. The classical techniques for studying controllability and reachability need to be further developed to understand these highly under actuated control problems of infinite dimensional systems.

4.4. Quantum probability, filtering and feedback

The models considered in previous sections pertain to open-loop control, and here we wish to provide a brief introduction to real-time feedback control of open quantum systems. To begin with we should clarify that we consider setups in which the plant is an open quantum system while the sensors, controller and actuators can reasonably be modeled as classical devices. (Scenarios involving quantum-mechanical controllers have also been considered, for example by S. Lloyd and co-workers [113].) In the theory of real-time feedback control of open quantum systems, there remains a distinction between state- and output-feedback paradigms, but care must be taken to avoid 'improper' applications of state-feedback methodology. (In principle it could suffice at this point to state the fact that quantum physics forbids perfect and complete measurements of the state of any single quantum system, but we will attempt to provide a more operational explanation.) While direct state feedback can of course be investigated in a quantum setting as a purely theoretical exercise, or as a computational tool for the design of open loop controls, it never really provides a faithful representation of actual feedback interconnection. For reasons that we will discuss shortly, quantum feedback control is always essentially stochastic and one must generally have recourse to a separation principle. In experimental scenarios with low measurement sensitivity (low signal-to-noise ratio), the sensor noise can be so dominated by 'excess' noise that the state estimator never converges to the level of intrinsic quantum uncertainties. In such cases the filtering problem can effectively be treated classically, leading for example to certainty-equivalent control models in which there is quantum dynamics (in the response of the system to applied fields) but no measurement backaction. This type of approach is formally similar to state feedback and is in fact well-motivated in current research on feedback cooling and closed-loop system identification of atomic ensembles [34, 114].

In experimental scenarios with high measurement sensitivity, however, it is crucial to utilize the type of quantum filtering equations that have been derived by researchers in mathematical physics [115] and quantum optics [116, 117]. (In intriguing recent work, M. James [118] has also derived quantum risk-sensitive filtering equations that could be utilized for the design and implementation of robust feedback controllers.) These equations are derived by considering a 'physical' account of the continuous measurement of an open quantum system (e.g., a cloud

of atoms) in which some probe field (*e.g.*, a laser beam)—itself a quantum system—is coupled to the plant via Hamiltonian dynamics (*e.g.*, electromagnetic coupling of atoms and photons according to Maxwell's Equations). This dynamical coupling creates correlations between the quantum states of the plant and the probe, such that a subsequent destructive measurement of the probe (*e.g.*, photodetection of the transmitted laser beam) yields some information about the evolving plant state. If it is assumed that such a sequence occurs repeatedly in coarse-grained time steps, one can take an Itô-like limit to obtain stochastic differential equations (SDE's) for propagating a recursive estimate of the plant state. It is important to note that quantum uncertainties associated with the probe field induce some degree of unavoidable randomness in the measurement (*e.g.*, photodetector) signals and/or the probe-induced perturbations of the plant evolution. Because of the quantum nature of the probe field it is impossible to conduct measurements on an open quantum system in such a way that both the sensor noise and 'measurement-induced process noise' vanish, and it is also impossible to make simultaneous accurate determinations of both noises 'after the fact' by scrutinizing the transmitted probe field. (There have been some theoretical investigations [119, 120] of schemes in which an optical probe beam is prepared in a highly 'squeezed' state to suppress sensor noise, while photodetection and feedback are used to cancel the measurement-induced process noise, but at present they are practically infeasible.) The use of proper quantum filtering equations in the design and analysis of quantum feedback systems is thus crucial to ensure full compliance with subtle physical constraints on achievable performance.

While it remains an outstanding research challenge to derive and to validate quantum filtering equations for solid-state quantum control systems, they are known with confidence for many systems in atomic physics including single-atom cavity QED [121] and hyperfine spin dynamics in atomic ensembles [122]. Such stochastic master equations (as they are known in quantum optics and atomic physics) have been used for numerical investigations of proposed quantum feedback schemes [47, 123] and also provide a starting point for rigorous analyses. Some scenarios of great practical interest, such as feedback control of atomic spin-squeezing [54] and closed-loop magnetometry [10], fall into a class of quantum Linear Quadratic Gaussian (LQG) systems for which exact analytic treatments are possible [124, 125]. For these systems the quantum filtering equations can be used to derive closed sets of SDE's for the first and second moments of a quorum of quantum variables. These SDE's can be put in the form of Kalman filters [126] and the usual LQG analyses from classical control theory apply straightforwardly. In such LQG quantum control models the only signature of the underlying quantum mechanics lies in the fact that certain inequalities must be observed among gain and covariance matrices therein; hence quantum LQG models are in a sense a subset of all possible classical LQG models [125].

Beyond the LQG regime it becomes difficult to obtain exact results, although some recent progress has been made on applying stochastic global [26] and almost-global [127] stability methods to solve stabilization problems in systems of low dimension. The basic state of affairs in nonlinear quantum control reflects the relatively underdeveloped state of nonlinear stochastic classical control, and one hopes that quantum systems will provide new impetus for a reinvigoration of the latter field as well.

4.5. Quantum system identification

As mentioned above, the problem of determining the structure of a protein using NMR is an example of what engineers might call a system identification problem. Applications in quantum metrology (such as magnetic field detection or inertial sensing) may also be viewed in a system identification framework. System identification problems have been widely studied in the field of automatic control because the design of an effective feedback control system begins with an accurate model, and because the use of open- or closed-loop controls can often improve identification accuracy or speed. Quantum system identification problems present new mathematical structure and optimization criteria because of the nature of the dynamics, some novel technical constraints, and the types of measurement backaction issues described in the preceding section.

It is useful to distinguish between quantum system identification procedures that are 'single-shot' versus those that employ a sequence of measurements on a fixed apparatus. As an example of the former type of problem, we refer back to our previous mention of LQG quantum feedback control on atomic systems [54]. It is possible to formulate extended Kalman filters for such scenarios, in which one or more parameters appearing in the Hamiltonian are treated as static or dynamic variables to be estimated from a continuous measurement signal. Some general investigations have appeared on the sensitivity and optimization of such procedures (including analytic studies in the Gaussian framework and numerical studies allowing more general likelihood functions) [128, 129, 130]. A thorough analysis has been performed of using this strategy for broadband magnetometry with atoms [10], and it has been shown that real-time feedback can be exploited for significant gains in robustness. Generally speaking it seems that closed-loop single-shot procedures provide an ideal approach to estimating non-stationary system parameters robustly.

While single-shot procedures will presumably become more prevalent in the future (with high-profile applications such as LIGO), most quantum system identification problems considered to date are based on the statistical analysis of a series of measurements on a fixed apparatus. The existing literature on classical system identification is almost exclusively devoted to problems for which the choice of input can be decoupled from the identification problem. But with insensitive techniques such as NMR, for which measurement time is precious, the design of input signals that reduce the time required for system identification is extremely important. Some recent work in this area [131] examines the problem of determining a good probing signal for system identification as a problem in minimizing the entropy of the probability density for the parameter values, given the observations [131]. This results in a mathematical formulation of the optimal input problem, that, at least in principle, has a solution that defines best input sequences or family of sequences that lead to efficient reduction of uncertainty in system parameters. (Note that in the literature of quantum information theory, this type of problem has been labeled 'quantum process tomography'.)

The problems of Hamiltonian identification also arise in other applications of quantum control. As mentioned above, there is now extensive experimental work on using closed loop methods for design of laser excitations in control of molecular reactions. These methods use stochastic search techniques, including genetic algorithms to learn control designs that optimize the final yield of the experiment [132, 133, 134]. Many of these problems could benefit by a systematic development of techniques of system identification for Hamiltonian estimation.

A complementary problem to system identification that often arises in quantum contexts is

that of state reconstruction. The basic challenge is to derive an optimal measurement [135] or (possibly adaptive) sequence [114] of measurements to be performed on one or more 'copies' of a quantum state in order to identify it as quickly and as accurately as possible. This identification make have any prior over a discrete or continuous set of possible states. The problem is clearly related to observability on one hand and communication theory on the other, providing an interesting possible point of contact between control theory and quantum networks [136].

5. Conclusions

There are now a number of quantum control systems for which basic theory is in place and experiment has reached an advanced stage of development. The study of these systems in control-theoretic terms will be important for a wide range of strategic applications. Broader engagement by the controls community could be exceptionally fruitful at this time, as could be the training of physicists with deeper knowledge of estimation, control and dynamical systems theories from engineering. Quantum control provides a unique opportunity for reexamining the physical basis of control and estimation theory, and may ultimately shed new light on fundamental issues in quantum physics as well.

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14. ABSTRACT The grant supported a workshop, held at Caltech in August 2004, that brought together experts in quantum mechanics, control theory, and dynamical systems for an exchange of ideas on the analysis, control, and design of quantum systems. One of the major goals of the workshop was to establish substantive technical interactions between physicists working on quantum 'applications' and control and dynamical systems researchers who have insights and tools but lack a concrete sense of what problems are of primary interest. The workshop highlighted anticipated applications of quantum control in quantum information science, control of molecular reactions, and design of electronic and photonic nanostructures. The workshop results are available on the web and documented in a paper that has been submitted to the International Journal of Robust and Nonlinear Control.					
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