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Principles and applications of control in quantum systems

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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), 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 behaviour 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 © 2005 John Wiley & Sons, Ltd.

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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 begins to see

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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, Belavkin, Rabitz and Tarn each reviewed seminal work dating back to the 1980s [1–3]. 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 PRACQSYS 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 manifestly non-classical phenomena are observable only under special laboratory conditions. Roughly speaking, quantum 'behaviour' 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 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 behaviour at room temperature (as in experiments on atomic ensembles and 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 behaviour 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 behaviour to appear classical, or at least imperfectly quantum.

The accurate quantitative modelling of 'imperfectly quantum' behaviour 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 behaviour 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 analyse 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 nuclei. 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 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 modelling 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 [6–8] 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 [11–13], 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.

Looking across these applications some common theoretical themes and challenges emerge. Many experiments, such as those in NMR, involve the simultaneous manipulation of an ensemble of systems with non-negligible dispersion in important physical parameters. The control challenge is to find excitations that are robust to such inhomogeneities. These problems naturally motivate 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 models raise interesting controllability issues that are discussed in Section 4.3.

Optimal control problems also arise naturally for quantum systems. Generally speaking, controls that achieve their objective in minimum time are desired to minimize dissipative effects associated with residual couplings to the system's environment. From a mathematical perspective, 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 previously been studied in great detail, rich new mathematical structures can be found in quantum problems. The added structure enables complete characterization of time-optimal trajectories and reachable sets for some of these systems [21, 22], as described in Section 4.1. Another class of quantum optimal control problem is steering in the presence of relaxation, as discussed in Section 4.2. Recent work of this type has shown, e.g. that significant improvements can be made in the sensitivity of multidimensional NMR experiments [23–25].

Research on *closed-loop* quantum control has opened new areas in estimation and filtering. 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 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

Here we provide brief overviews of three relevant classes of experimental systems. 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. Tutorial introductions are beyond the scope of this article, so our aim is to provide references in a manner that highlights points of interest to the controls community.

3.1. Magnetic resonance

NMR began as a tool for characterizing organic molecules but has spread to diverse areas including pharmaceutics, structural biology, solid state chemistry, condensed matter physics, rheology and medical diagnostics (medical resonance imaging) [27–29]. The principles of NMR are a paradigm for further physical methods that rely on interactions between radiation and matter. It is thus not surprising that NMR experiments also serve as good model problems for quantum control. In this section we briefly introduce NMR studies of biomolecular structure and describe some associated control problems.

Modern NMR experiments use a large static magnetic field $B_z \sim 5 - 20$ T to orient the magnetic moments of atomic nuclei. The resulting net magnetization $\mathbf{M}$ in the direction of B_z is then manipulated by an oscillating radio frequency field $(B_x(t), B_y(t))$ in a plane perpendicular to B_z. This field exerts a torque on $\mathbf{M}$, which then evolves as

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix} = \gamma \begin{bmatrix} 0 & -B_z & B_y(t) \\ B_z & 0 & -B_x(t) \\ -B_y(t) & B_x(t) & 0 \end{bmatrix} \begin{bmatrix} M_x \\ M_y \\ M_z \end{bmatrix} \tag{1}$$

The Bloch model in Equation (1) is a model bilinear control system where the time varying $(B_x(t), B_y(t))$ act as controls. Since $(B_x(t), B_y(t))/B_z \lesssim 10^{-4}$, subtle design principles must be employed.

In a typical scenario, oscillating $(B_x(t), B_y(t))$ can be used to transfer initial magnetization $\mathbf{M}(0) = (0, 0, 1)$, to the x–y plane. If the oscillating field is then turned off, $\mathbf{M}$ precesses freely around B_z at the Larmor frequency ω_0. This induces an oscillating current in a nearby coil, which when Fourier transformed shows a peak at $\omega_0 = \gamma B_z$, where γ depends upon nuclear species. At a field of 14 T, the Larmor frequencies of protons (^{1}H), nitrogen (^{15}N) and carbon (^{13}C) are 600, 60 and 150 MHz, respectively. NMR thus provides an important analytical tool in chemistry as spectral peaks reveal the atomic composition of molecules. In addition, the detailed electronic environment of a nucleus alters its local magnetic field and hence shifts its Larmor frequency. These shifts are characteristic of the chemical environment of the spins and can be used to assign the various peaks in a proton spectrum to specific amino acids of a protein ('frequency labelling') [30, 31]. Following this, a series of measurements can be used to characterize interactions among the frequency labelled protons to yield information on distances between the amino acids. These constraints can be sufficient to determine the protein structure (folding configuration).

The spectrum of a large protein is poorly resolved due to crowding of the spectrum by numerous resonances and increased line widths caused by relaxation. Multidimensional NMR can be used [27] to counteract this. Multidimensional NMR experiments generate a two dimensional spectrum, where each peak in the spectrum is labelled by the 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 species coupled to it (such as ^{15}N). As a result, two protons with overlapping Larmor frequencies can now be distinguished by their associated nitrogen frequencies. Experiments that generate such two-dimensional spectra involve intricate control of coupled spin dynamics [27, 31]; in NMR spectroscopy of proteins, many elaborate procedures have been developed to improve resolution [31].

There are many intriguing problems related to optimizing the sensitivity of multidimensional NMR. From the perspective of control theory, these are related to steering bilinear systems with drift. Finding time-optimal pulse sequences that induce a certain evolution of coupled spins or reach a target state with minimum relaxation losses are long-standing problems in NMR. They have only recently been addressed from a control theory perspective [21–25], and there are many other open problems that can benefit from similar treatments. Optimal control of coupled spin topologies has a direct connection to quantum information, as will be discussed in Sections 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 isolated from bulk matter, gas-phase atoms provide a canonical setting for validating elementary methodology. Techniques have been developed for controlling electron orbital motion and hyperfine spin dynamics, with potential applications in quantum information processing and metrology. The development of laser cooling techniques has made it possible to observe and to induce quantum phenomena in atomic centre-of-mass motion 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 developed previously by atomic physicists are mainly of intuitive origin (often adapted from magnetic resonance [28, 29]). But researchers working on atomic systems have begun to explore the utility of robust pulse sequences from NMR [32] and of optimal control theory [33] 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 many atomic physics experiments). As it is often possible to model atomic systems essentially from first principles, sophisticated synthesis techniques from control theory could have significant impact. Preliminary investigations suggest that model complexity can be a serious obstacle, however, as can technical limitations on generating laser control fields. Atomic dynamical timescales can be quite short ($\sim 10^{-9}$ to $\sim 10^{-3}$ s), which presents a challenge for the implementation of closed-loop methods. Model reduction and robustness 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 modelling 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 modelled, thus enabling a rigorous treatment of the quantum-mechanical measurement 'backaction' in quantum feedback control (see Section 4.4).

Several 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. Long coherence times can be obtained with trapped ions, 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 analysed from the perspective of geometric control theory [38, 39]. Trapped ions have provided some of the most sophisticated examples of open-loop quantum control to date, but 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 (see however References [40, 41]). For practical applications this could be less of an impediment than one might imagine, however, as stochastic perturbations can be kept relatively small in these experiments and high purity initial states can be prepared.

Many of the attractive features of trapped ions can also be found in single-atom cavity quantum electrodynamics (cavity QED) [42]. In modern cavity QED, 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). Optical cavity QED has the benefit of being the one of the few 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 on 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 quantum control of cavity QED was stimulated by applications in quantum information science, and also by general interest 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 vapour cell samples, in which special technical preparations enable long coherence times for collective internal degrees of freedom of gas-phase atoms whose centre-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 Sections 4.4 and 4.5).

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 the 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 centre-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 neighbouring atoms in the lattice [32, 61–63]. 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 rich dynamical settings for the investigation of quantum phenomena. The construction of accurate theoretical models 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 only briefly survey some systems that were discussed at the PRACQSYS workshop and provide experimental and theoretical references. It seems worth noting that recent work on solid state quantum control suggests that 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 quantum information processing. It is now possible to produce coherent superpositions of quantum states of such circuits, to observe coherent dynamics in them, and to perform readout with high fidelity and low backaction [68]. Open-loop control in superconducting circuits is thus reaching a level of maturity comparable to that of trapped ion systems, although the decoherence mechanisms are much less well understood and the achieved control fidelities have accordingly been substantially lower. But superconducting circuits provide access to a broader range of dynamical phenomena, including bifurcations and limit-cycle behaviour 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 open exciting new prospects for observing conditional evolution and possibly implementing real-time feedback control.

Electron spin degrees of freedom in semiconductor systems are likewise amenable to quantum control, with important 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 gains in speed and miniaturization. One 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 one would think of using pulsed magnetic fields, but this would be very difficult to do with the required speeds and localization. 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 cantilevers with extremely low internal dissipation and weak environmental couplings, combined with state-of-the-art cryogenics and electro-mechanical sensors, has made it possible to approach conditions in which quantum behaviour should become observable and controllable. Initial theoretical studies have been conducted of the feasibility of using feedback for active cooling of a cantilever to its quantum mechanical ground state [74], and strategies have been proposed and analysed [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 system 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

Quantum control typically involves actuation via tailored electromagnetic fields. These are then bilinear control problems (usually with drift) for the unitary evolution operator U, which (neglecting decoherence) evolves under the Schrödinger equation ($\hbar = 1$)

$$\dot{U} = -i\left[H_d + \sum_{j=1}^{m} u_j H_j\right] U \tag{2}$$

H_d is the internal Hamiltonian of the system and H_j are the Hamiltonians describing responses to applied controls (usually electromagnetic fields) $u_j(t)$. There has been significant interest in controllability of these systems [76–86] both in finite dimensions (as in the case of coupled spins) and infinite dimensions (as in the cases of trapped ions and of molecular dynamics [38, 39, 85]).

In the finite dimensional case results on controllability carry over from classical control theory [87–89], as captured by the Lie algebra $\{-iH_d, -iH_j\}_{\mathrm{LA}}$ generated by the Hamiltonians H_d and H_i. For infinite-dimensional bilinear control systems, many conceptual and technical difficulties remain [38, 39]. Controllability arguments for steering infinite dimensional systems between eigenstates have been primarily constructive [90, 91]. There has been recent interest in utilizing geometric control theory but much work remains to be done. Infinite-dimensional bilinear control problems also arise naturally when one is trying to steer an ensemble of finite dimensional quantum systems [92–95], as discussed in Section 4.3.

In general, external excitations must cooperate with the intrinsic dynamics H_d to achieve a desired evolution, such as transferring coherence between spins in magnetic resonance [21]. This reliance on H_d puts a fundamental limit on the time required to implement a desired evolution. 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]. This problem has practical significance since time-optimal methods for steering the system in Equation (2) between points of interest minimize dissipative effects caused by interaction with the environment.

Recent study of such problems has elucidated the relationship between Lie algebras generated by control Hamiltonians $\mathfrak{k} = \{-iH_j\}_{\mathrm{LA}}$ and the full control algebra $\mathfrak{g} = \{-iH_d, -iH_j\}_{\mathrm{LA}}$ and the associated groups $K = \exp(\mathfrak{k})$ and $G = \exp(\mathfrak{g})$ [21]. The time required to synthesize a desired evolution in Equation (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 contexts of magnetic resonance and quantum information processing with spin-$\frac{1}{2}$ particles [21, 22, 78], where the space G of unitary transformation of coupled spins is $SU(4)$. External excitations produce local unitary transformations in the subgroup $K = SU(2) \otimes SU(2)$. Analysis of the resulting control systems on $SU(4)/SU(2) \otimes SU(2)$ [21, 96, 97] has made the synthesis of unitary transformations for coupled spin-$\frac{1}{2}$ particles ('qubits') transparent. The associated Cartan decomposition of $SU(4)$ in terms of the subgroup $SU(2) \otimes SU(2)$ has been utilized for design of quantum logic gates [76, 96, 98–101]. Many of the entanglement-generation properties of quantum gates can be studied using these Cartan decompositions [101]. The reachable sets and time-optimal controls in Equation (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 [102, 103].

Geometric methods hold promise for problems of optimal control 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 [104] on homogeneous spaces [22]. In the general problem of control of a network of coupled qubits, the control subgroup $K = SU(2) \otimes SU(2) \otimes \cdots SU(2)$ of local unitary transformations is much smaller than the group of all unitary transformations $G = SU(2^n)$. Finding efficient ways to realize unitary evolutions in a network of coupled quantum systems is thus an interesting and timely challenge for geometric control theory. 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 [105].

Although study of bilinear control systems is not new, physical problems arising in control of quantum systems motivate new mathematical structures and facilitate further developments in 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 its evolution non-unitary and induces relaxation to some equilibrium state. In applications, this leads to loss of signal and information. Manipulating quantum systems in a manner that minimizes relaxation losses is a fundamental challenge of practical importance.

There has been significant interest in the development of techniques for optimal control of quantum dynamics in the presence of relaxation, primarily in the context of magnetic resonance [23–25, 106, 107]. Most of the work in this area has focused on scenarios where the environment can be approximated as an infinite thermostat and the evolution of the open quantum system can be modelled by an equation of the Lindblad type [108, 109],

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

The evolution is no longer unitary but the control system retains a bilinear structure as $\rho \to L(\rho)$ is a trace preserving linear map. Understanding controllability properties of systems of the form 3 is a topic of active investigation [110].

Consider a model problem associated with optimal control of coupled spin dynamics in the presence of relaxation [24]. Given the control system [111]

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 & -u & 0 & 0 \\ u & -k & -J & 0 \\ 0 & J & -k & -v \\ 0 & 0 & v & 0 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \tag{4}$$

with $k, J > 0$, and 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? Note that even if the strength of controls is unbounded, there is a fundamental limit on the maximum value of x_4.

The study of problems on control of open quantum systems has led to the investigation of certain constraint bilinear control problems of the following form [24, 111]. Let $x \in \mathbb{R}^n$

and $u \in \mathbb{R}^m$. Consider the system

$$\dot{x} = \left(A + \sum_i^k f_i(u) B_i\right) x \tag{5}$$

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_o. 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 [112, 113].

4.3. *Control of ensembles*

Many quantum control applications involve simultaneous steering of a large ensemble of systems with a single applied control. In practice, the elements of the ensemble can vary in physical parameters that govern their dynamics. In magnetic resonance experiments, e.g. the spins of an ensemble may have large dispersion in their Larmor frequencies, strength of couplings between coupled spin pairs and spin relaxation rates [114]. 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 [92–95]. From the standpoint of mathematical control, the challenge is to simultaneously control a continuum of systems with the same control.

Consider the following bilinear control system that captures the dynamics of an ensemble of spin-$\frac{1}{2}$ particles in an external magnetic field, as described in Section 3.1

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 & -\omega & -au(t) \\ \omega & 0 & av(t) \\ au(t) & -av(t) & 0 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{6}$$

Consider now the problem of designing controls $u(t)$ and $v(t)$ that simultaneously steer an ensemble of such systems with $\omega \in [-B, B]$ from an initial state $(x, y, z) = (0, 0, 1)$ to a final state $(x, y, z) = (1, 0, 0)$ [92]. 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 [92]. In Equation (6), the parameter a might also show dispersion. In magnetic resonance applications, this arises when different spatial positions in the sample experience different rf-fields due to field inhomogeneities.

These problems raise questions about controllability, i.e. showing that there exists a control law $(u(t), v(t))$ satisfying $\sqrt{u^2(t) + v^2(t)} \leqslant A_{\max}$ which simultaneously steers all the systems with $\omega \in [-B, B]$ and $a \in [1 - \varepsilon, 1 + \varepsilon]$ to a ball of chosen radius around the final state $(1, 0, 0)$ in finite time. Furthermore, practical considerations like relaxation (Section 3.1) motivate construction of the shortest control that achieves this goal. These are problems of 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 Equation (6) is relevant in NMR and MRI applications.

Another type of problem that arises in ensemble quantum control is the optimization of an average quantity. Consider the model problem of optimal state transfer in the presence of relaxation described in Equation (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. that maximize

$$\int_{J_1}^{J_2} \int_{k_1}^{k_2} x_4(J, k, t)\, \mathrm{d}J\, \mathrm{d}k$$

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 modelled classically. (Scenarios involving quantum-mechanical controllers have also been considered, e.g. by Lloyd and co-workers [115].) In the theory of real-time quantum feedback control, 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. As discussed below, quantum feedback control is essentially stochastic and one must generally resort to a separation principle. However, 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, 116].

In experimental scenarios with high measurement sensitivity it is crucial to utilize quantum filtering equations as have been derived by researchers in mathematical physics [117] and quantum optics [118, 119]. (In intriguing recent work, James [120] has derived quantum risk-sensitive filtering equations that could be utilized for robust feedback control.) 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 (SDEs) 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 [121, 122] 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 [123] and hyperfine spin dynamics in atomic ensembles [124]. 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, 125] and also provide a starting point for analytic work. 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 [126, 127]. 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 can be put in the form of Kalman filters [128] 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 [127].

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 [129] 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 an 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) [130–132]. 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 [133] 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 [133]. 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 labelled '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 [134–136]. 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 [137] or (possibly adaptive) sequence [116] 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 may 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 [138].

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. The control-theoretic study of these systems 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. 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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